Access DB# 108971

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: *Maury Audet* Examiner #: *79808* **Date:** 11/01/03
Art Unit: *1654* Phone Number: *305-5039* **Serial Number:** 10/039317
Mail Box & Bldg/Room Locat.: CM1-*11D13; 11D04* Results Format Preferred: *PAPER*

If more than one search is submitted, please prioritize searches in order of need.

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Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: _____

Inventors (please provide full names): _____

Earliest Priority Filing Date: 10/23/00

For Sequence Searches Only *Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Please search just the compound of

1) EXAMPLE 34

2) If found, search w/ for treatment of "any virus" & more specifically "Hepatitis C Virus or HCV"

3) Inventor Search-1 (E. Scott Priestley).

Tx, MAURY

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STAFF USE ONLY	Type of Search	Vendors and cost where applicable
Searcher: Sapna Patel	NA Sequence (#)	STN
Searcher Phone #: 308-4419	AA Sequence (#)	Dialog
Searcher Location	Structure (#)	Questel/Orbit
Date Searcher Picked Up:	Bibliographic	Dr.Link
Date Completed: 11/3/03	Litigation	Lexis/Nexis
Searcher Prep & Review Time:	Fulltext	Sequence Systems
Clerical Prep Time:	Patent Family	WWW/Internet
Online Time:	Other	Other (specify)

PTO-1590 (8-01)

=> fil hcaplus
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FILE COVERS 1907 - 21 Nov 2003 VOL 139 ISS 22
FILE LAST UPDATED: 20 Nov 2003 (20031120/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

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L1 19 SEA FILE=HCAPLUS ABB=ON PLU=ON "PRIESTLEY E"/AU OR ("PRIESTLE
Y E SCOTT"/AU OR "PRIESTLEY E SCOTT"/IN) OR ("PRIESTLEY ELDON
SCOTT"/AU OR "PRIESTLEY ELDON SCOTT"/IN)

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=> d ibib abs l1 1-19

L1 ANSWER 1 OF 19 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2003:290802 HCAPLUS
DOCUMENT NUMBER: 139:176419
TITLE: Selection of a thiazole urea-resistant variant of bovine viral diarrhea virus that maps to the RNA-dependent RNA polymerase
AUTHOR(S): King, Robert W.; Scarnati, Helen T.; **Priestley, E. Scott**; De Lucca, Indawati; Bansal, Anu; Williams, J. Kendall
CORPORATE SOURCE: The Experimental Station, Bristol-Myers Squibb, Wilmington, DE, USA
SOURCE: Antiviral Chemistry & Chemotherapy (2002), 13(5), 315-323
CODEN: ACCHEH; ISSN: 0956-3202
PUBLISHER: International Medical Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB By passing wild type bovine viral diarrhea virus (BVDV) in increasing concns. of DPC-A69280-29, a thiazole urea class compd. that inhibits BVDV replication, we were able to select several variants of BVDV that exhibited decreased susceptibility to this compd. When the non-structural genes of these variants were sequenced and compared with wild type, only one change was common to all the variants that also exhibited resistance to DPC-A69280-29 (>10-fold increase in IC50). This change was a T-to-A transversion at position 11198 of the BVDV genome, which would cause a

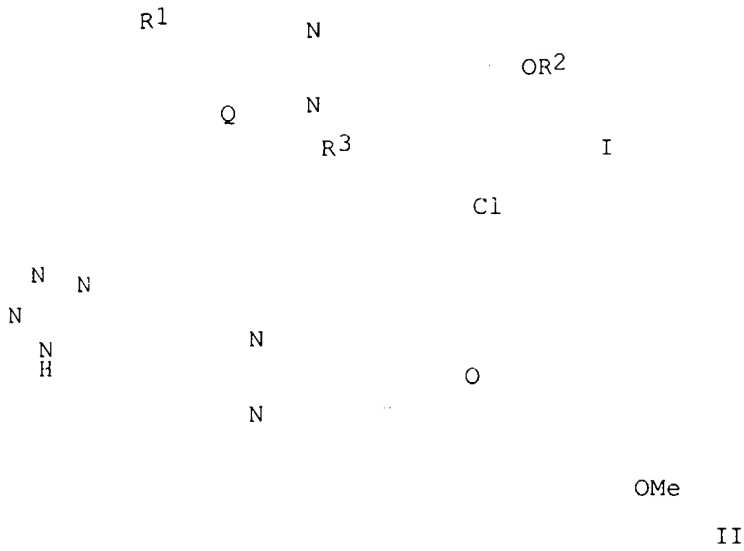
predicted substitution of isoleucine for phenylalanine at amino acid 78 of the RNA-dependent RNA polymerase (RdRp). This substitution would occur in a region of the BVDV RdRp which has been proposed to be important for the formation of the RdRp homodimer that is essential for the activity of the enzyme. However, since DPC-69280-29 inhibits BVDV replication by interfering with the initiation of viral RNA synthesis, we discuss the possibility that this region of the BVDV RdRp also may play a role in the initiation process. Furthermore, since this region is located fairly close to the template RNA, we also propose that the role it plays may involve either template selection, stabilization or processivity.

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 2 OF 19 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2003:261620 HCAPLUS
DOCUMENT NUMBER: 138:287673
TITLE: Preparation of phenylbenzimidazole compounds useful for treating hepatitis C virus
INVENTOR(S): **Priestley, Eldon Scott**; Decicco, Carl P.; Hudyma, Thomas W.; Zheng, Xiaofan
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 74 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003026587	A2	20030403	WO 2002-US30989	20020926
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003134853	A1	20030717	US 2002-259041	20020926

PRIORITY APPLN. INFO.: US 2001-324874P P 20010926
OTHER SOURCE(S): MARPAT 138:287673
GI



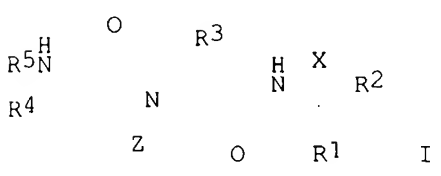
II

AB Compds. of formula I [Q = CH, N; R1 = tetrazolyl, MeCONHSO2, PhCONHSO2, etc.; R2 = CH2-aryl, CHPh2, etc.; R3 = cycloalkyl] are prepd. which are useful in treating viral hepatitis C. Thus, II was prepd. and had an IC50 of 0.14 .mu.M against HCV NS5B RdRp (RNA-dependent RNA polymerase).

L1 ANSWER 3 OF 19 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2003:23525 HCAPLUS
DOCUMENT NUMBER: 138:90078
TITLE: Preparation of lactam acylaminoalkaneboronates as inhibitors of hepatitis C virus NS3 protease.
INVENTOR(S): **Priestley, E. Scott**; Decicco, Carl P.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 45 pp., Cont.-in-part of U.S. Ser. No. 626,286, abandoned.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003008828	A1	20030109	US 2001-10184	20011206

PRIORITY APPLN. INFO.: US 1999-145631P P 19990726
US 2000-626286 B2 20000725
OTHER SOURCE(S): MARPAT 138:90078
GI



AB Title compds. I [X = B(OH)2, BY1Y2, COCONHR1a; Y1, Y2 = OH, F, amino,

alkoxy; BY1Y2 = atoms to form a cyclic boron ester, amide, or amide-ester contg. 2-20 C atoms and optionally 1-3 N, O, or S atoms; R1, R1a = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl; R2 = H; R1R2C = cycloalkyl; R3 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, Ph, naphthyl, heteroaryl; R4 = H, (substituted) alkyl, Ph, PhCH2, PhCH2CH2; R5 = H, QR5a; Q = chain of 0-3 amino acids; R5a = SOR6, SO2R6, COR6, CO2R8, etc.; R6 = (substituted) alkyl, Ph, naphthyl, PhCH2, heteroaryl; R8 = alkyl, PhCH2, cycloalkylmethyl; Z = (CH2)1-3} were prepd. as inhibitors of hepatitis C virus NS3 protease. Thus, (1R)-1-[[(2S)-3-cyclohexyl-2-[3-isopropyl-3-[[(2S)-3-methyl-2-[(2-pyrazinylcarbonyl)amino]butanoyl]amino]-2-oxo-1-pyrrolidinyl]propanoyl]amino]-3-butenylboronic acid (+)-pinanediol ester was prepd. by soln. phase chem. A no. of I inhibited hepatitis C virus NS3 protease with Ki <60 .mu.M.

L1 ANSWER 4 OF 19 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:907216 HCAPLUS
DOCUMENT NUMBER: 138:4821
TITLE: Preparation of peptide inhibitors of hepatitis C virus NS3 protein
INVENTOR(S): **Priestley, E. Scott**
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 54 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002177725	A1	20021128	US 2001-39317	20011028
PRIORITY APPLN. INFO.:			US 2000-242557P P	20001023

OTHER SOURCE(S): MARPAT 138:4821
AB The invention relates to a novel class of peptides R3-A-N(R2)CHR1-W [W = B(OH)2 or a deriv., COCO-Q, COCONH-Q, COCO2-Q, COCF2CONH-Q, COCF3, COCF2CF3, or CHO, where Q is an amino acid residue or an alkyl, alkenyl, or alkynyl radical substituted by CO2H, SO2H, SO3H, PO2H, PO3H (or their esters), etc.; A is a (di- through hepta)peptide residue; R1 = R1a(CH2)2-6 (R1a = substituted phenyl), BuCH2, BuCH2CH2, Me3C(CH2)3, Et2CH(CH2)3, or 3-cyclobutylpropyl; R2 = H, alkyl, aryl, arylalkyl, or cycloalkyl; R3 = H, alkyl, aryl, arylalkyl, COR11, CO2R11, CONHR11, SOR11, SO2R11 (R11 = alkyl, aryl, or heterocyclyl which may be substituted), or an NH2-blocking group} which are useful as serine protease inhibitors, more particularly as hepatitis C virus (HCV) NS3 protease inhibitors. Thus, H-Asp-Glu-Val-Val-Pro-(R)-amino(phenyl)methylboronic acid (+)-pinanediol ester was prepd. by soln. phase chem. Compds. of the invention were found to exhibit a Ki of .ltoreq. 50 .mu.M, thereby confirming their utility as effective HCV NS3 protease inhibitors.

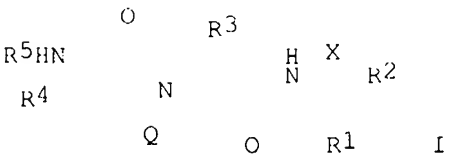
L1 ANSWER 5 OF 19 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:767330 HCAPLUS
DOCUMENT NUMBER: 138:221813
TITLE: P1 Phenethyl peptide boronic acid inhibitors of HCV NS3 protease
AUTHOR(S): **Priestley, E. Scott**; De Lucca, Indawati; Ghavimi, Bahman; Erickson-Viitanen, Susan; Decicco, Carl P.
CORPORATE SOURCE: Experimental Station, Bristol-Myers Squibb Pharmaceutical Research Institute, Wilmington, DE, 19880-0500, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(21), 3199-3202
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A series of peptide boronic acids contg. extended, hydrophobic P1 residues was prepd. to probe the shallow, hydrophobic S1 region of HCV NS3 protease. The p-trifluoromethylphenethyl P1 substituent was identified as optimal with respect to inhibitor potency for NS3 and selectivity against elastase and chymotrypsin.
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 6 OF 19 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:78359 HCAPLUS
DOCUMENT NUMBER: 134:147855
TITLE: Preparation of lactam acylaminoalkaneboronates as inhibitors of hepatitis C virus NS3 protease.
INVENTOR(S): **Priestley, E. Scott**; Decicco, Carl P.
PATENT ASSIGNEE(S): Du Pont Pharmaceuticals Company, USA
SOURCE: PCT Int. Appl., 130 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001007407	A1	20010201	WO 2000-US20189	20000726
W: AU, BR, CA, CN, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1206449	A1	20020522	EP 2000-950642	20000726
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				

PRIORITY APPLN. INFO.: US 1999-145631P P 19990726
WO 2000-US20189 W 20000726
OTHER SOURCE(S): MARPAT 134:147855
GI



AB Title compds. [I; X = B(OH)2, BYY1, COCONHR1a; Y1, Y2 = OH, F, amino, alkoxy; BY1Y2 = atoms to form a cyclic boron ester, amide, or amide-ester contg. 2-20 C atoms and optionally 1-3 N, O, or S atoms; R1, R1a = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl; R2 = H; R1R2C = cycloalkyl; R3 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, Ph, naphthyl, heteroaryl; R4 = H, (substituted) alkyl, Ph, PhCH2, PhCH2CH2; R5 = H, QR5a; Q = chain of 0-3 amino acids; R5a = SOR6, SO2R7, COR6, CO2R8; R6 = (substituted) alkyl, Ph, naphthyl, PhCH2, heteroaryl; R7 = H, alkyl; R8 = alkyl, PhCH2, cycloalkylmethyl; Q = (CH2)1-3], were prepd. Thus, (1R)-1-[[(2S)-3-cyclohexyl-2-[3-isopropyl-3-[[(2S)-3-methyl-2-[(2-pyrazinylcarbonyl)amino]butanoyl]amino]-2-oxo-1-pyrrolidinyl]propanoyl]amino]-3-butenylboronic acid (+)-pinanediol ester

was prepd. by soln. phase chem. A no. of I inhibited hepatitis C virus NS3 protease with Ki<60 .mu.M.
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 7 OF 19 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:607748 HCAPLUS
DOCUMENT NUMBER: 133:335259
TITLE: 1-Aminocyclopropaneboronic Acid: Synthesis and Incorporation into an Inhibitor of Hepatitis C Virus NS3 Protease
AUTHOR(S): **Priestley, E. Scott**; Decicco, Carl P.
CORPORATE SOURCE: Department of Chemical and Physical Sciences, DuPont Pharmaceuticals Company, Wilmington, DE, 19880, USA
SOURCE: Organic Letters (2000), 2(20), 3095-3097
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:335259
AB The previously unreported .alpha.,.alpha.-disubstituted 1-aminoboronate esters have potential utility in peptidomimetic design, particularly against serine protease targets. A concise synthesis of 1-aminocyclopropaneboronate pinanediol ester is reported, and a peptidyl deriv. has modest affinity (Ki = 1.6 .mu.M) for hepatitis C NS3 protease. Analogs with iso-Pr and cyclohexyl in place of cyclopropyl were also prepd. and tested.
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 8 OF 19 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:410768 HCAPLUS
DOCUMENT NUMBER: 131:144777
TITLE: Design and Synthesis of New Amino Glycoside Antibiotics Containing Neamine as an Optimal Core Structure: Correlation of Antibiotic Activity with in Vitro Inhibition of Translation
AUTHOR(S): Greenberg, William A.; **Priestley, E. Scott**; Sears, Pamela S.; Alper, Phil B.; Rosenbohm, Christoph; Hendrix, Martin; Hung, Shang-Cheng; Wong, Chi-Huey
CORPORATE SOURCE: Department of Chemistry and Skaggs Institute of Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Journal of the American Chemical Society (1999), 121(28), 6527-6541
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The structure and activity of the pseudo-disaccharide core found in amino glycoside antibiotics was probed with a series of synthetic analogs in which the position of amino groups was varied around the glucopyranose ring. The naturally occurring structure neamine was the best in the series according to assays for in vitro RNA binding and antibiotic activity. With this result in hand, neamine was used as a common core structure for the synthesis of new antibiotics, which were evaluated for binding to models of the Escherichia coli 16S A-site rRNA, in vitro protein synthesis inhibition, and antibiotic activity. Anal. of RNA binding revealed some correlation between the relative affinity and specificity of RNA binding and antibacterial efficacy. However, the correlation was not linear. This result led us to develop the in vitro translation assay in an effort to better understand amino glycoside-RNA

interactions. A linear correlation between in vitro translation inhibition and antibiotic activity was obsd. In addn., IC50s in the protein synthesis assay were typically lower than the Kds obtained for RNA binding, suggesting that binding of these compds. to intact ribosomes is tighter in these cases than binding to the model RNA oligodeoxyribonucleotides. This reflects possible differences in RNA conformation between intact ribosomes and the free RNA of the model system, or possible high-affinity ribosomal binding sites in addn. to the A-site RNA.

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 9 OF 19 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1998:503937 HCAPLUS
DOCUMENT NUMBER: 129:225287
TITLE: Specificity of aminoglycoside antibiotics for the A-site of the decoding region of ribosomal RNA
AUTHOR(S): Wong, Chi-Huey; Hendrix, Martin; **Priestley, E. Scott**; Greenberg, William A.
CORPORATE SOURCE: Dep. Chem. and the Skaggs Inst. Chem. Biol., The Scripps Res. Inst., La Jolla, CA, 92037, USA
SOURCE: Chemistry & Biology (1998), 5(7), 397-406
CODEN: CBOLE2; ISSN: 1074-5521
PUBLISHER: Current Biology Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Aminoglycoside antibiotics bind to the A-site of the decoding region of 16S RNA in the bacterial ribosome, an interaction that is probably responsible for their activity. A detailed study of the specificity of aminoglycoside binding to A-site RNA would improve our understanding of their mechanism of antibiotic activity. We have studied the binding specificity of several aminoglycosides with model RNA sequences derived from the 16S ribosomal A-site using surface plasmon resonance. The 4,5-linked (neomycin) class of aminoglycosides showed specificity for wild-type A-site sequences, but the 4,6-linked class (kanamycins and gentamicins), generally showed poor specificity for the same sequences. Methylation of a cytidine in the target RNA, as found in the Escherichia coli ribosome, had negligible effects on aminoglycoside binding. Although both 4,5- and 4,6-linked aminoglycosides target the same ribosomal site, they appear to bind and effect antibiotic activity in different manners. The aminoglycosides might recognize different RNA conformations or the interaction might involve different RNA tertiary structures that are not equally sampled in our ribosome-free model. These results imply that models of rRNA must be carefully designed if the data are expected to accurately reflect biol. activity.

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 10 OF 19 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1998:490647 HCAPLUS
DOCUMENT NUMBER: 129:136438
TITLE: Preparation of nucleic acid binders having a hydroxyamine motif as protein synthesis inhibitors
INVENTOR(S): Wong, Chi-huey; Hendrix, Martin; Alper, Phil; **Priestley, E. Scott**
PATENT ASSIGNEE(S): The Scripps Research Institute, USA
SOURCE: PCT Int. Appl., 244 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9830570	A1	19980716	WO 1998-US549	19980113
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9858219	A1	19980803	AU 1998-58219	19980113
US 6120997	A	20000919	US 1998-6597	19980113
PRIORITY APPLN. INFO.:			US 1997-35483P	P 19970113
			WO 1998-US549	W 19980113

OTHER SOURCE(S): MARPAT 129:136438

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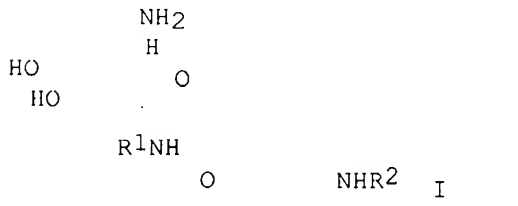

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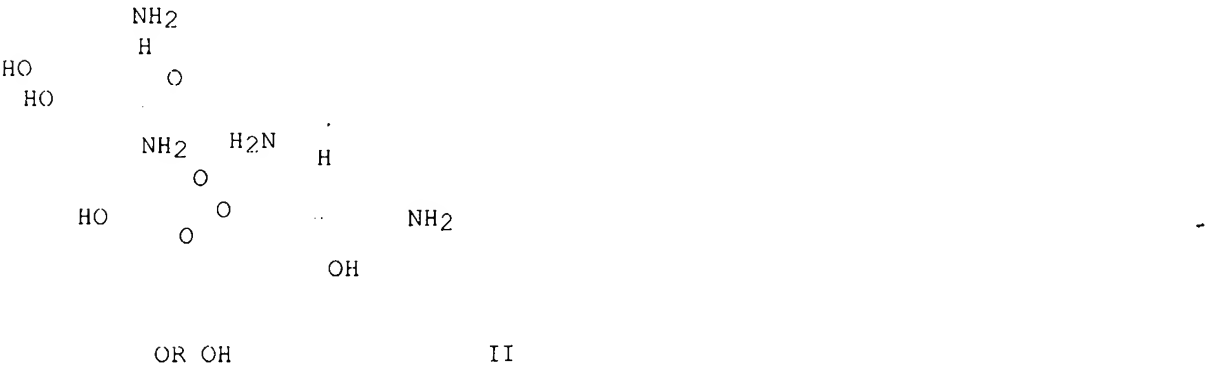


II

AB The invention relates to the combination of hydroxyamines with nucleic acid binding motifs to generate mols. and libraries of mols. targeting specific nucleic acid sequences. In particular, a series of libraries are constructed which contain hydroxyamine functionalities I (R1 = H, amide of amino acids; R2 = H, n-Pr, i-Pr, alkylamine, amide, hydroxyalkyl) that are attached to various template backbones which display varying degrees of mol. recognition to phosphodiesters and varying degrees of sequence specific recognition to nucleic acids. Thus, amino glycoside II was prepd. and showed antibacterial activity against E. coli (MIC = 18.5).

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

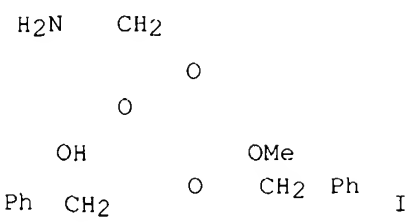
L1 ANSWER 11 OF 19 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:238376 HCAPLUS
DOCUMENT NUMBER: 126:287612
TITLE: Direct Observation of Aminoglycoside-RNA Interactions by Surface Plasmon Resonance
AUTHOR(S): Hendrix, Martin; **Priestley, E. Scott**; Joyce,

Gerald F.; Wong, Chi-Huey
CORPORATE SOURCE: Department of Chemistry, Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Journal of the American Chemical Society (1997), 119(16), 3641-3648
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The specificity of neomycin B and related aminoglycoside antibiotics in their interaction with the Rev responsive element (RRE) of HIV-1 mRNA has been studied by directly observing the aminoglycoside-RNA complexes using surface plasmon resonance. Several different RNA sequences, each with a biotin tag, have been prepd. using T7 RNA polymerase-catalyzed transcription of synthetic DNA templates and have been immobilized on a streptavidin-coated surface for the binding study. The results indicate that neomycin B is not specific for the G-rich bubble region in RRE. Rather, it appears to interact with three different sites, each with a submicromolar dissocn. const., within the 67-nucleotide domain II of RRE. Further anal. of neomycin B binding with three short synthetic RNA hairpins showed binding with submicromolar affinity and 1:1 stoichiometry in each case. This suggests that neomycin B may generally bind with this affinity to regular A-form RNA or hairpin loops. The approach described here is generally useful for understanding the fundamental interactions involved in the specific recognition of nucleic acids by small mols. which is the basis of rational drug design.

L1 ANSWER 12 OF 19 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:159007 HCAPLUS
TITLE: A chemical approach to aminoglycoside--RNA recognition
AUTHOR(S): **Priestley, E. Scott**; Hendrix, Martin; Alper, Phil B.; Park, William K. C.; Wong, Chi-Huey
CORPORATE SOURCE: Department Chemistry, Scripps Research Institute, La Jolla, CA, 92037, USA
SOURCE: Book of Abstracts, 213th ACS National Meeting, San Francisco, April 13-17 (1997), CARB-073. American Chemical Society: Washington, D. C.
CODEN: 64AOAA
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
AB The aminoglycoside antibiotics are one of the few classes of small mols. which bind to specific RNA sequences and modulate their biol. activity. Our efforts to understand these interactions have encompassed several approaches. Model studies have identified the 1,3-hydroxyamine structural motif, commonly found in aminoglycosides, as an excellent ligand for complexation of phosphate groups. A surface plasmon resonance based assay has been developed which allows direct observation of aminoglycoside binding to immobilized RNA transcripts. The results, for several biol. relevant sequences from HIV mRNA and prokaryotic rRNA, highlight specificity as a key issue in developing therapeutically useful aminoglycoside derivs. Finally, progress in the rational design-synthesis, and combinatorial synthesis of analogs with improved properties will be presented.

L1 ANSWER 13 OF 19 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:116805 HCAPLUS
DOCUMENT NUMBER: 126:225481
TITLE: Hydroxyamines as a new motif for the molecular recognition of phosphodiesters: implications for aminoglycoside-RNA interactions
AUTHOR(S): Hendrix, Martin; Alper, Phil B.; **Priestley, E. Scott**; Wong, Chi-Huey
CORPORATE SOURCE: Department Chemistry, Scripps Research Institute, La

Jolla, CA, 92037, USA
SOURCE: Angewandte Chemie, International Edition in English (1997), 36(1/2), 95-98
CODEN: ACIEAY; ISSN: 0570-0833
PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Prepn. of aminodeoxy glycosides, e.g. I, and their binding consts. to dimethylphosphate and hydrogen chloride are reported.
REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 14 OF 19 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1996:405975 HCAPLUS
DOCUMENT NUMBER: 125:168557
TITLE: Energetics of triple helix formation by oligodeoxyribonucleotides containing nonnatural bases (DNA, pyrimidines)
AUTHOR(S): **Priestley, Eldon Scott**
CORPORATE SOURCE: California Institute of Technology, Pasadena, CA, USA
SOURCE: (1996) 192 pp. Avail.: Univ. Microfilms Int., Order No. DA9617420
From: Diss. Abstr. Int., B 1996, 57(2), 1091
DOCUMENT TYPE: Dissertation
LANGUAGE: English
AB Unavailable

L1 ANSWER 15 OF 19 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:520654 HCAPLUS
DOCUMENT NUMBER: 123:163473
TITLE: Sequence Composition Effects on the Energetics of Triple Helix Formation by Oligonucleotides Containing a Designed Mimic of Protonated Cytosine
AUTHOR(S): **Priestley, E. Scott**; Dervan, Peter B.
CORPORATE SOURCE: Arnold and Mabel Beckman Laboratories of Chemical Synthesis, California Institute of Technology, Pasadena, CA, 91125, USA
SOURCE: Journal of the American Chemical Society (1995), 117(17), 4761-5
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A non-natural nucleoside, 1-(2-deoxy-.beta.-D-ribofuranosyl)-3-methyl-5-amino-1H-pyrazolo[4,3-d]pyrimidin-7-one (P), mimics protonated cytosine and specifically binds GC base pairs within a pyrimidine.cntdot.purine.cntdot.pyrimidine triple helix. Quant. footprint titrn. expts. at neutral pH (22 .degree.C, 100 mM NaCl, 10 mM bis-tris, 250 .mu.M spermine) now reveal dramatic sequence compn. effects on the

energetics of triple helix formation by oligonucleotides contg. P or 5-methylcytosine (mC). Purine tracts of sequence compn. 5'-d(AAAAAGAGAGAGAGA)-3' are bound by oligonucleotide 5'-d(TTTTTmCTmCTmCTmCTmCT)-3' 4 orders of magnitude more strongly than by 5'-d(TTTTTPTPTPTPTPT)-3' (KT .apprxeq. 3 .times. 109 M-1 and KT = 1 .times. 105 M-1, resp.). Conversely, purine tracts of sequence compn. 5'-d(AAAAGAAAAGGGGGGA)-3' are bound by oligonucleotide 5'-d(TTTTmCTTTTmCmCmCmCmCT)-3' 5 orders of magnitude less strongly than by 5'-d(TTTTmCTTTTPPPPPPT)-3' (KT < 5 .times. 104 M-1 and KT .apprxeq. 4 .times. 109 M-1, resp.). The complementary nature of P and mC expands the repertoire of G-rich sequences which may be targeted by triple helix formation.

L1 ANSWER 16 OF 19 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:397896 HCAPLUS
DOCUMENT NUMBER: 122:240324
TITLE: Design of an N7-Glycosylated Purine Nucleoside for Recognition of GC Base Pairs by Triple Helix Formation
AUTHOR(S): Hunziker, Juerg; **Priestley, E. Scott**; Brunar, Helmut; Dervan, Peter B.
CORPORATE SOURCE: Arnold and Mabel Beckman Laboratories of Chemical Synthesis, California Institute of Technology, Pasadena, CA, 91125, USA
SOURCE: Journal of the American Chemical Society (1995), 117(9), 2661-2
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Prepn. and equil. assocn. consts. of 20 triple helical oligodeoxyribonucleotide complexes for recognition of GC base pairs are reported.

L1 ANSWER 17 OF 19 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1993:664792 HCAPLUS
DOCUMENT NUMBER: 119:264792
TITLE: NMR structural studies on a nonnatural deoxyribonucleoside which mediates recognition of GC base pairs in pyrimidine.cntdot.purine.cntdot.pyrimidine DNA triplexes
AUTHOR(S): Radhakrishnan, Ishwar; Patel, Dinshaw J.; **Priestley, E. Scott**; Nash, Huw M.; Dervan, Peter B.
CORPORATE SOURCE: Coll. Physicians Surg., Columbia Univ., New York, NY, 10032, USA
SOURCE: Biochemistry (1993), 32(41), 11228-34
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
AB As a part of the authors' ongoing efforts to define the structural aspects of unusual pairing alignments in DNA triplexes by NMR spectroscopy, the authors have examd. the structural role of a nonnatural deoxyribonucleoside, P1, that has been shown to mediate the recognition of GC base paris in pyrimidine.cntdot.purine.cntdot.pyrimidine DNA triplexes. A qual. interpretation of the NMR data indicates that this analog of protonated cytosines is readily accommodated in the third strand segment of an intramol. triplex system. Furthermore, the obsd. NOE patterns position the imino and amino protons of P1 opposite the N7 and O6 atoms of guanine, resp., consistent with the previously proposed pairing scheme.

L1 ANSWER 18 OF 19 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1992:40928 HCAPLUS
DOCUMENT NUMBER: 116:40928

TITLE: Methylenecyclopropanecarboxylates and -dicarboxylates, efficient reagents for the [3+2] methylenecyclopentane annulation of unactivated and electron-rich alkenes

AUTHOR(S): Singleton, Daniel A.; Huval, Chad C.; Church, Kevin M.; **Priestley, E. Scott**

CORPORATE SOURCE: Dep. Chem., Texas A and M Univ., College Station, TX, 77843, USA

SOURCE: Tetrahedron Letters (1991), 32(41), 5765-8
CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 116:40928

GI

CMe_2 CMe_2

CO_2Me

CO_2Me I CO_2Et II

AB The readily available methylenecyclopropanes I and II efficiency annulate unactivated and electron-rich alkenes via a thiyl-radical catalyzed chain cyclization.

L1 ANSWER 19 OF 19 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1929:46484 HCAPLUS

DOCUMENT NUMBER: 23:46484

ORIGINAL REFERENCE NO.: 23:5322a-b

TITLE: The analysis of union materials

AUTHOR(S): Lloyd, L. L.; **Priestley, E.**

SOURCE: Journal of the Society of Dyers and Colourists (1929), 45, 201-4
CODEN: JSDCAA; ISSN: 0037-9859

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB Cotton-asbestos mixts. were conditioned, treated 24 hrs. cold with 35% on vol. H2SO4 (80.degree. tw.), washed acid-free, reconditioned and weighed. For cotton, regenerated cellulose rayons and wool, the samples were conditioned and weighed, rayon was extd. with 69.degree. tw. H2SO4 (30% by vol. acid) 20 min. at 50.degree., washed thoroughly in water with squeezing, conditioned and weighed. Cotton was removed by using 69.degree. tw. H2SO4 24 hrs. at 25.degree.. The residue was washed thoroughly, conditioned and weighed. Cotton may also be removed by ammoniacal Cu hydroxide (see Krais and Blitz, Ibid 36, 228(1920); cf. C. A. 14, 3535). Acetate rayons may be removed by acetone extn. Some portions of dyed acetate rayons, dissected out, are insol. in acetone. For rayon-silk mixts., more study is required for undischarged or heavily basic dyed material. Discharged silk is resistant to 21.degree. tw. HCl for 15 min. whereas regenerated celluloses dissolve. This method appears to work well with cotton, rayon and wool mixts.

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6 C     4 C
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  10

STEREO ATTRIBUTES: NONE
L24         2473 SEA FILE=REGISTRY SSS FUL L22
L26         2925 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L24
L27            6 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L26(L)(?VIRUS? OR ?VIRAL? OR
                 ?VIRUST? OR VIRICI?)


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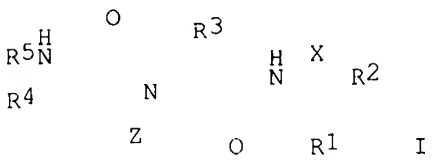
L27  ANSWER 1 OF 6  HCAPLUS  COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:         2003:23525  HCAPLUS
DOCUMENT NUMBER:          138:90078
```

TITLE: Preparation of lactam acylaminoalkaneboronates as inhibitors of hepatitis C virus NS3 protease.
INVENTOR(S): Priestley, E. Scott; Decicco, Carl P.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 45 pp., Cont.-in-part of U.S. Ser. No. 626,286, abandoned.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003008828	A1	20030109	US 2001-10184	20011206

PRIORITY APPLN. INFO.: US 1999-145631P P 19990726
US 2000-626286 B2 20000725
OTHER SOURCE(S): MARPAT 138:90078
GI



AB Title compds. I [X = B(OH)2, BY1Y2, COCONHR1a; Y1, Y2 = OH, F, amino, alkoxy; BY1Y2 = atoms to form a cyclic boron ester, amide, or amide-ester contg. 2-20 C atoms and optionally 1-3 N, O, or S atoms; R1, R1a = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl; R2 = H; R1R2C = cycloalkyl; R3 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, Ph, naphthyl, heteroaryl; R4 = H, (substituted) alkyl, Ph, PhCH2, PhCH2CH2; R5 = H, QR5a; Q = chain of 0-3 amino acids; R5a = SOR6, SO2R6, COR6, CO2R8, etc.; R6 = (substituted) alkyl, Ph, naphthyl, PhCH2, heteroaryl; R8 = alkyl, PhCH2, cycloalkylmethyl; Z = (CH2)1-3] were prepd. as inhibitors of hepatitis C virus NS3 protease. Thus, (1R)-1-[[(2S)-3-cyclohexyl-2-[3-isopropyl-3-[[(2S)-3-methyl-2-[(2-pyrazinylcarbonyl)amino]butanoyl]amino]-2-oxo-1-pyrrolidinyl]propanoyl]amino]-3-butenylboronic acid (+)-pinanediol ester was prepd. by soln. phase chem. A no. of I inhibited hepatitis C virus NS3 protease with Ki <60 .mu.M.

IT **18680-27-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of lactam acylaminoalkaneboronates as inhibitors of hepatitis C **virus** NS3 protease)

L27 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:907216 HCAPLUS
DOCUMENT NUMBER: 138:4821
TITLE: Preparation of peptide inhibitors of hepatitis C virus NS3 protein
INVENTOR(S): Priestley, E. Scott
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 54 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002177725	A1	20021128	US 2001-39317	20011028

PRIORITY APPLN. INFO.: US 2000-242557P P 20001023
OTHER SOURCE(S): MARPAT 138:4821

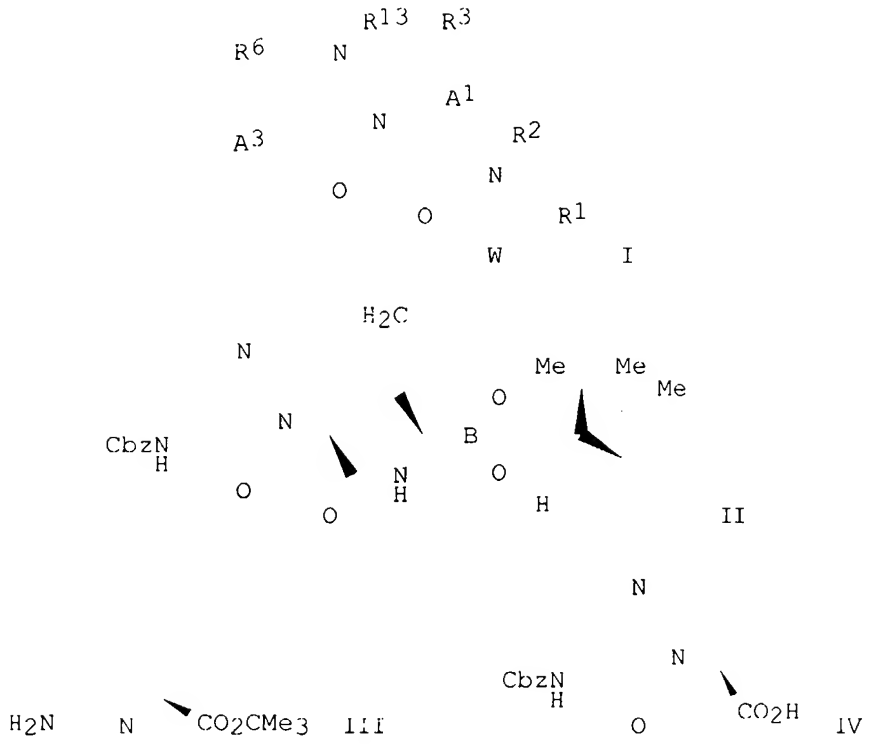
AB The invention relates to a novel class of peptides R3-A-N(R2)CHR1-W [W = B(OH)2 or a deriv., COCO-Q, COCONH-Q, COCO2-Q, COCF2CONH-Q, COCF3, COCF2CF3, or CHO, where Q is an amino acid residue or an alkyl, alkenyl, or alkynyl radical substituted by CO2H, SO2H, SO3H, PO2H, PO3H (or their esters), etc.; A is a (di- through hepta)peptide residue; R1 = R1a(CH2)2-6 (R1a = substituted phenyl), BuCH2, BuCH2CH2, Me3C(CH2)3, Et2CH(CH2)3, or 3-cyclobutylpropyl; R2 = H, alkyl, aryl, arylalkyl, or cycloalkyl; R3 = H, alkyl, aryl, arylalkyl, COR11, CO2R11, CONHR11, SOR11, SO2R11 (R11 = alkyl, aryl, or heterocyclyl which may be substituted), or an NH2-blocking group] which are useful as serine protease inhibitors, more particularly as hepatitis C virus (HCV) NS3 protease inhibitors. Thus, H-Asp-Glu-Val-Val-Pro-(R)-amino(phenyl)methylboronic acid (+)-pinanediol ester was prepd. by soln. phase chem. Compds. of the invention were found to exhibit a Ki of .ltoreq. 50 .mu.M, thereby confirming their utility as effective HCV NS3 protease inhibitors.

IT **18680-27-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of peptide inhibitors of hepatitis C **virus** NS3 protein)

L27 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:465982 HCAPLUS
DOCUMENT NUMBER: 137:47213
TITLE: Preparation of fused pyrimidinones and benzodioxaborolidinylpropylaminopyrrolo[1,2-a]pyrimidines as inhibitors of hepatitis C ns3 protease for the treatment of hepatitis C and other viral diseases
INVENTOR(S): Glunz, Peter W.; Douty, Brent D.; Han, Wei
PATENT ASSIGNEE(S): Bristol-Myers Squibb Pharma Company, USA
SOURCE: PCT Int. Appl., 270 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002048116	A2	20020620	WO 2001-US47911	20011212
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002030763	A5	20020624	AU 2002-30763	20011212
US 2003064962	A1	20030403	US 2001-15304	20011212

PRIORITY APPLN. INFO.: US 2000-255290P P 20001213
WO 2001-US47911 W 20011212
OTHER SOURCE(S): MARPAT 137:47213
GI



II

III

IV

AB Fused pyrimidinones I [A1 = (un)substituted CH2, CH2CH2, CH2CH2CH2, A2CH2, A2CH2CH2, CH2A2CH2; A2 = O, S, (un)substituted imino; A3 = H, R9CO, R9O, R9S, R9CONH, R9NHCO, etc.; W = (un)substituted boronic acid ester, QCOCO, QNHCOCO, QOCOCO, QNHCOCF2CO, COQ3, F3CCO, F3CCF2CO, OHC, amino acid residue; Q3 = (un)substituted aryl, heterocyclyl; R1 = H, F, (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl; R2 = H, alkyl; Q, R3, R9 = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclyl; R6, R13 = H, (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, aralkyl, cycloalkylalkyl; R3R13 = (un)substituted carbocyclic ring, alkylidene] and particularly dioxaborolylpropylamino pyrrolopyriminecarboxamides such as II are prepd. as inhibitors of hepatitis C viral protein ns3 protease for the treatment of hepatitis C and other viral diseases. E.g., esterification of L-pyroglutamic acid with AcOCMe3 and HClO4, thionation with Lawesson's reagent, S-methylation with MeI, and amidation with NH4Cl gives nonracemic aminopyrrolinecarboxylate III. Treatment of III with di-Me 2-(methoxymethylene)malonate, hydrolysis of the Me ester moiety with LiOH, prepn. of the acyl azide with diphenylphosphoryl azide and Curtius rearrangement in the presence of PhCH2OH, and hydrolysis of the tert-Bu ester with CF3CO2H gives pyrrolo[1,2-a]pyrimidine IV. Coupling of IV with an .alpha.-allyl aminomethylboronate pinanediol ester gives II. I inhibit hepatitis C ns3 protease with IC50 values of <100 .mu.M. Pharmaceutical compns. contg. I are given.

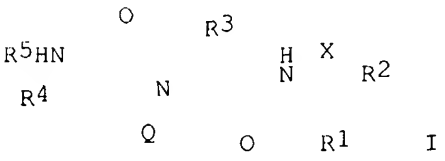
IT **18680-27-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; prepn. of fused pyrimidinones and benzodioxaborolidinylpropylaminopyrrolo[1,2-a]pyrimidines as inhibitors of hepatitis C ns3 protease for the treatment of hepatitis C and other **viral** diseases)

L27 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:78359 HCAPLUS

DOCUMENT NUMBER: 134:147855
TITLE: Preparation of lactam acylaminoalkaneboronates as inhibitors of hepatitis C virus NS3 protease.
INVENTOR(S): Priestley, E. Scott; Decicco, Carl P.
PATENT ASSIGNEE(S): Du Pont Pharmaceuticals Company, USA
SOURCE: PCT Int. Appl., 130 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001007407	A1	20010201	WO 2000-US20189	20000726
W: AU, BR, CA, CN, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1206449	A1	20020522	EP 2000-950642	20000726
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				

PRIORITY APPLN. INFO.: US 1999-145631P P 19990726
WO 2000-US20189 W 20000726
OTHER SOURCE(S): MARPAT 134:147855
GI



AB Title compds. [I; X = B(OH)2, BYY1, COCONHR1a; Y1, Y2 = OH, F, amino, alkoxy; BY1Y2 = atoms to form a cyclic boron ester, amide, or amide-ester contg. 2-20 C atoms and optionally 1-3 N, O, or S atoms; R1, R1a = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl; R2 = H; R1R2C = cycloalkyl; R3 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, Ph, naphthyl, heteroaryl; R4 = H, (substituted) alkyl, Ph, PhCH2, PhCH2CH2; R5 = H, QR5a; Q = chain of 0-3 amino acids; R5a = SOR6, SO2R7, COR6, CO2R8; R6 = (substituted) alkyl, Ph, naphthyl, PhCH2, heteroaryl; R7 = H, alkyl; R8 = alkyl, PhCH2, cycloalkylmethyl; Q = (CH2)1-3], were prepd. Thus, (1R)-1-[[(2S)-3-cyclohexyl-2-[3-isopropyl-3-[[(2S)-3-methyl-2-[(2-pyrazinylcarbonyl)amino]butanoyl]amino]-2-oxo-1-pyrrolidinyl]propanoyl]amino]-3-butenylboronic acid (+)-pinanediol ester was prepd. by soln. phase chem. A no. of I inhibited hepatitis C virus NS3 protease with Ki<60 .mu.M.

IT **18680-27-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of lactam acylaminoalkaneboronates as inhibitors of hepatitis C **virus** NS3 protease)

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L27 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:31525 HCAPLUS

DOCUMENT NUMBER: 134:101193
TITLE: Preparation of peptide boronic acid inhibitors of hepatitis C virus protease
INVENTOR(S): Kettner, Charles A.; Jagannathan, Sharada; Forsyth, Timothy Patrick
PATENT ASSIGNEE(S): Du Pont Pharmaceuticals Company, USA
SOURCE: PCT Int. Appl., 258 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001002424	A2	20010111	WO 2000-US18655	20000707
WO 2001002424	A3	20010719		
W: AU, BR, CA, CN, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 2000057888	A5	20010122	AU 2000-57888	20000707
EP 1196436	A2	20020417	EP 2000-943413	20000707
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				

PRIORITY APPLN. INFO.: US 1999-142561P P 19990707
WO 2000-US18655 W 20000707
OTHER SOURCE(S): MARPAT 134:101193

AB .alpha.-Aminoboronic acids and corresponding peptide analogs R3-A-NR2CHR1BY1Y2 [Y1, Y2 = OH, F, an amino group, alkoxy or BY1Y2 is a cyclic boron ester, amide or amide-ester; R1 = CH:CH2, CH2CH:CH2, CH:CHCH3, C.tplbond.CH, C.tplbond.CCH3, CH2C.tplbond.CH, cyclopropyl, cyclopropylmethyl, cyclobutyl, cyclobutylmethyl, mercaptoalkyl, alkyldithioalkyl, etc.; A is a bond, a natural or unnatural amino acid residue, or a peptide residue comprising 2-10 amino acids; R2 = H, alkyl, aryl, arylalkyl, cycloalkyl; R3 = H, alkanoyl, alkyl, alkenyl, alkynyl, aryl, carbalkoxy, alkylsulfinyl, alkylsulfonyl, carbamoyl, etc.] were prepd. for the treatment of hepatitis C viral infections. Thus, Boc-Asp(OBu-t)-Glu(OBu-t)-Val-Val-Pro-boroCpa-OH pinanediol ester (Boc = tert-butoxycarbonyl, boroCpa is L-2-amino-3-cyclopropylboronic acid residue) was prepd. by std. methods of peptide coupling in soln. Enzyme assays, dosages and formulations are discussed.

IT **18680-27-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of peptide boronic acid inhibitors of hepatitis C **virus** protease)

L27 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:683497 HCAPLUS
DOCUMENT NUMBER: 132:44640
TITLE: Synthesis and antiviral and cytostatic activities of carbocyclic nucleosides incorporating a modified cyclobutane ring. Part 1. Guanosine analogues
AUTHOR(S): Figueira, M. Jose; Blanco, J. Manuel; Caamano, Olga; Fernandez, Franco; Garcia-Mera, Xerardo; Lopez, Carmen; Andrei, Graciela; Snoeck, Robert; Padalko, Elisabeth; Neyts, Johan; Balzarini, Jan; De Clercq, Erik
CORPORATE SOURCE: Departamento Quimica Organica, Facultad Farmacia, Univ. Santiago, Santiago de Compostela, E-15706, Spain
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1999), 332(10), 348-352

CODEN: ARPMAS; ISSN: 0365-6233
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:44640
AB Five carbocyclic nucleosides were prepd. by constructing a guanine or 8-azaguanine base on the amino group of (1'S,3'R)-3-(3'-amino-2',2'-dimethylcyclobutyl)-1-propanol, and their activities against a variety of viruses and tumor cell lines were detd. Two of the compds. showed a detectable activity at subtoxic concns. against some viruses tested.
IT **24903-95-5**, Nopinone
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of cyclobutane-derived guanosine analogs with antitumor and **antiviral** activity)
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> select hit rn l27 1-6
E1 THROUGH E2 ASSIGNED

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STRUCTURE FILE UPDATES: 20 NOV 2003 HIGHEST RN 619253-33-7
DICTIONARY FILE UPDATES: 20 NOV 2003 HIGHEST RN 619253-33-7

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

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Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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=> s e1-e2
1 18680-27-8/BI
(18680-27-8/RN)
1 24903-95-5/BI
(24903-95-5/RN)
L28 2 (18680-27-8/BI OR 24903-95-5/BI)

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=> d ide can l28 1-2

L28 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2003 ACS on STN
RN **24903-95-5** REGISTRY
CN Bicyclo[3.1.1]heptan-2-one, 6,6-dimethyl- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Norpinanone, 6,6-dimethyl- (6CI, 7CI, 8CI)
OTHER NAMES:
CN .beta.-Pinone
CN 6,6-Dimethylbicyclo[3.1.1]heptan-2-one
CN Nopinone
CN NSC 135004
FS 3D CONCORD
DR 473-60-9, 30469-48-8
MF C9 H14 O
CI COM
LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, IFICDB, IFIPAT, IFIUDB, NAPRALERT, SPECINFO, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

223 REFERENCES IN FILE CA (1907 TO DATE)
223 REFERENCES IN FILE CAPLUS (1907 TO DATE)
10 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 139:323666

REFERENCE 2: 139:296264

REFERENCE 3: 139:264676

REFERENCE 4: 139:117042

REFERENCE 5: 139:100048

REFERENCE 6: 139:89114

REFERENCE 7: 139:39360

REFERENCE 8: 138:406566

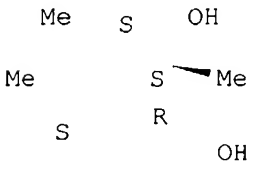
REFERENCE 9: 138:390516

REFERENCE 10: 138:78235

L28 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2003 ACS on STN
RN **18680-27-8** REGISTRY
CN Bicyclo[3.1.1]heptane-2,3-diol, 2,6,6-trimethyl-, (1S,2S,3R,5S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2,3-Pinanediol, (1S,2S,3R,5S)-(+)- (8CI)
CN Bicyclo[3.1.1]heptane-2,3-diol, 2,6,6-trimethyl-, [1S-

(1.alpha.,2.alpha.,3.alpha.,5.alpha.)]-
OTHER NAMES:
CN (1S,2S,3R,5S)-(+)-Pinane-2,3-diol
CN (1S,2S,3R,5S)-(+)-Pinanediol
CN (1S,2S,3R,5S)-2,3-Pinanediol
CN 2.alpha.,3.alpha.-Pinanediol
FS STEREOSEARCH
MF C10 H18 O2
CI COM
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX, CSCHEM, GMELIN*, MSDS-OHS, SPECINFO, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry. Rotation (+).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

110 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
111 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:338034

REFERENCE 2: 139:323591

REFERENCE 3: 139:100818

REFERENCE 4: 139:69373

REFERENCE 5: 138:362119

REFERENCE 6: 138:338495

REFERENCE 7: 138:338491

REFERENCE 8: 138:221813

REFERENCE 9: 138:165634

REFERENCE 10: 138:165629

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L37              STR

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                        23
     22  21  20
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                         O
                        17 5C       C 4


NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  19

STEREO ATTRIBUTES: NONE
L39         4335 SEA FILE=REGISTRY SSS FUL L37
L43        85305 SEA FILE=REGISTRY ABB=ON  PLU=ON  BORON?
L45       306461 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L43 OR ?BORON?
L46         2074 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L39
L47           17 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L46 AND L45


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=> d ibib abs hitrn 147 1-17

L47  ANSWER 1 OF 17  HCAPLUS  COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:         2003:23525  HCAPLUS
DOCUMENT NUMBER:          138:90078
TITLE:                    Preparation of lactam acylaminoalkaneboronates
                          as inhibitors of hepatitis C virus NS3 protease.
INVENTOR(S):              Priestley, E. Scott; Decicco, Carl P.
PATENT ASSIGNEE(S):       USA
SOURCE:                   U.S. Pat. Appl. Publ., 45 pp., Cont.-in-part of U.S.
                          Ser. No. 626,286, abandoned.
                          CODEN: USXXCO
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   2
PATENT INFORMATION:

     PATENT NO.        KIND  DATE          APPLICATION NO.  DATE
     ---------------   ----  --------      ---------------  --------
     US 2003008828      A1   20030109      US 2001-10184    20011206
PRIORITY APPLN. INFO.:                   US 1999-145631P  P  19990726
                                         US 2000-626286   B2 20000725
OTHER SOURCE(S):          MARPAT 138:90078
GI
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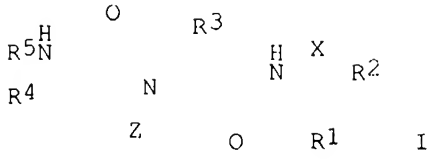


AB Title compds. I [X = B(OH)2, BY1Y2, COCONHR1a; Y1, Y2 = OH, F, amino, alkoxy; BY1Y2 = atoms to form a cyclic **boron** ester, amide, or amide-ester contg. 2-20 C atoms and optionally 1-3 N, O, or S atoms; R1, R1a = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl; R2 = H; R1R2C = cycloalkyl; R3 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, Ph, naphthyl, heteroaryl; R4 = H, (substituted) alkyl, Ph, PhCH2, PhCH2CH2; R5 = H, QR5a; Q = chain of 0-3 amino acids; R5a = SOR6, SO2R6, COR6, CO2R8, etc.; R6 = (substituted) alkyl, Ph, naphthyl, PhCH2, heteroaryl; R8 = alkyl, PhCH2, cycloalkylmethyl; Z = (CH2)1-3] were prepd. as inhibitors of hepatitis C virus NS3 protease. Thus, (1R)-1-[[(2S)-3-cyclohexyl-2-[3-isopropyl-3-[[(2S)-3-methyl-2-[(2-pyrazinylcarbonyl)amino]butanoyl]amino]-2-oxo-1-pyrrolidinyl]propanoyl]amino]-3-**butenylboronic** acid (+)-pinanediol ester was prepd. by soln. phase chem. A no. of I inhibited hepatitis C virus NS3 protease with Ki <60 .mu.M.

IT **323196-93-6P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of lactam **acylaminoalkaneboronates** as inhibitors of hepatitis C virus NS3 protease)

IT **204765-53-7**
RL: PRP (Properties)
(unclaimed sequence; prepn. of lactam **acylaminoalkaneboronates** as inhibitors of hepatitis C virus NS3 protease.)

L47 ANSWER 2 OF 17 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:907216 HCAPLUS
DOCUMENT NUMBER: 138:4821
TITLE: Preparation of peptide inhibitors of hepatitis C virus NS3 protein
INVENTOR(S): Priestley, E. Scott
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 54 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002177725	A1	20021128	US 2001-39317	20011028

PRIORITY APPLN. INFO.: US 2000-242557P P 20001023
OTHER SOURCE(S): MARPAT 138:4821
AB The invention relates to a novel class of peptides R3-A-N(R2)CHR1-W [W = B(OH)2 or a deriv., COCO-Q, COCONH-Q, COCO2-Q, COCF2CONH-Q, COCF3, COCF2CF3, or CHO, where Q is an amino acid residue or an alkyl, alkenyl, or alkynyl radical substituted by CO2H, SO2H, SO3H, PO2H, PO3H (or their esters), etc.; A is a (di- through hepta)peptide residue; R1 = R1a(CH2)2-6 (R1a = substituted phenyl), BuCH2, BuCH2CH2, Me3C(CH2)3, Et2CH(CH2)3, or 3-cyclobutylpropyl; R2 = H, alkyl, aryl, arylalkyl, or cycloalkyl; R3 = H, alkyl, aryl, arylalkyl, COR11, CO2R11, CONHR11, SOR11, SO2R11 (R11 = alkyl, aryl, or heterocyclyl which may be substituted), or an NH2-blocking group] which are useful as serine protease inhibitors, more particularly

as hepatitis C virus (HCV) NS3 protease inhibitors. Thus, H-Asp-Glu-Val-Val-Pro-(R)-amino(phenyl)**methylboronic** acid (+)-pinanediol ester was prepd. by soln. phase chem. Compds. of the invention were found to exhibit a Ki of .ltoreq. 50 .mu.M, thereby confirming their utility as effective HCV NS3 protease inhibitors.

IT **274918-51-3P**
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of peptide inhibitors of hepatitis C virus NS3 protein)

IT **476333-92-3P 476333-93-4P 476333-94-5P**
476333-95-6P 476333-96-7P 476333-97-8P
476333-98-9P 476333-99-0P 476334-00-6P
476334-01-7P 476334-02-8P 476334-03-9P
476334-04-0P 476334-05-1P 476334-06-2P
476334-07-3P 476334-08-4P 476334-10-8P
476334-11-9P 476334-12-0P 476334-13-1P
476334-14-2P 476334-15-3P 476334-16-4P
476334-17-5P 476334-24-4P 476334-25-5P
476334-26-6P 476334-27-7P 476334-28-8P
476334-29-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of peptide inhibitors of hepatitis C virus NS3 protein)

IT **98-80-6**, Phenylboric acid **5419-55-6**, Triisopropyl borate **5720-05-8**, 4-**Methylphenylboronic** acid **5720-07-0**, 4-**Methoxyphenylboronic** acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of peptide inhibitors of hepatitis C virus NS3 protein)

IT **76110-78-6P 99429-45-5P 99429-46-6P**
289709-75-7P 319011-74-0P 319011-76-2P
319012-18-5P 476334-32-4P 476334-34-6P
476334-38-0P 476334-42-6P 476334-46-0P
476334-77-7P 476335-12-3P 476335-16-7P
476335-17-8P 476335-20-3P 476335-24-7P
476335-28-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of peptide inhibitors of hepatitis C virus NS3 protein)

L47 ANSWER 3 OF 17 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:767330 HCAPLUS
DOCUMENT NUMBER: 138:221813
TITLE: P1 Phenethyl peptide **boronic** acid inhibitors of HCV NS3 protease
AUTHOR(S): Priestley, E. Scott; De Lucca, Indawati; Ghavimi, Bahman; Erickson-Viitanen, Susan; Decicco, Carl P.
CORPORATE SOURCE: Experimental Station, Bristol-Myers Squibb Pharmaceutical Research Institute, Wilmington, DE, 19880-0500, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(21), 3199-3202
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of peptide **boronic** acids contg. extended, hydrophobic P1 residues was prepd. to probe the shallow, hydrophobic S1 region of HCV NS3 protease. The p-trifluoromethylphenethyl P1 substituent was identified as optimal with respect to inhibitor potency for NS3 and selectivity against elastase and chymotrypsin.

IT **500763-17-7P 500763-19-9P 500763-21-3P**

500763-23-5P 500763-25-7P 500763-27-9P
500763-29-1P 500763-31-5P 500763-33-7P
500763-35-9P 500763-37-1P 500763-39-3P
500763-42-8P 500763-44-0P 500763-46-2P
500763-48-4P 500763-50-8P 500763-52-0P
500763-53-1P 500763-55-3P 500763-57-5P
500763-59-7P 500763-61-1P 500763-63-3P
500763-65-5P 500763-67-7P 500763-69-9P
500763-71-3P 500763-73-5P 500763-74-6P
500763-75-7P 500763-76-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of P1 phenethyl peptide **boronic** acid inhibitors of HCV NS3 protease)

IT **98-80-6, Phenylboronic** acid **5419-55-6,**
Triisopropyl borate **274918-51-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of P1 phenethyl peptide **boronic** acid inhibitors of HCV NS3 protease)

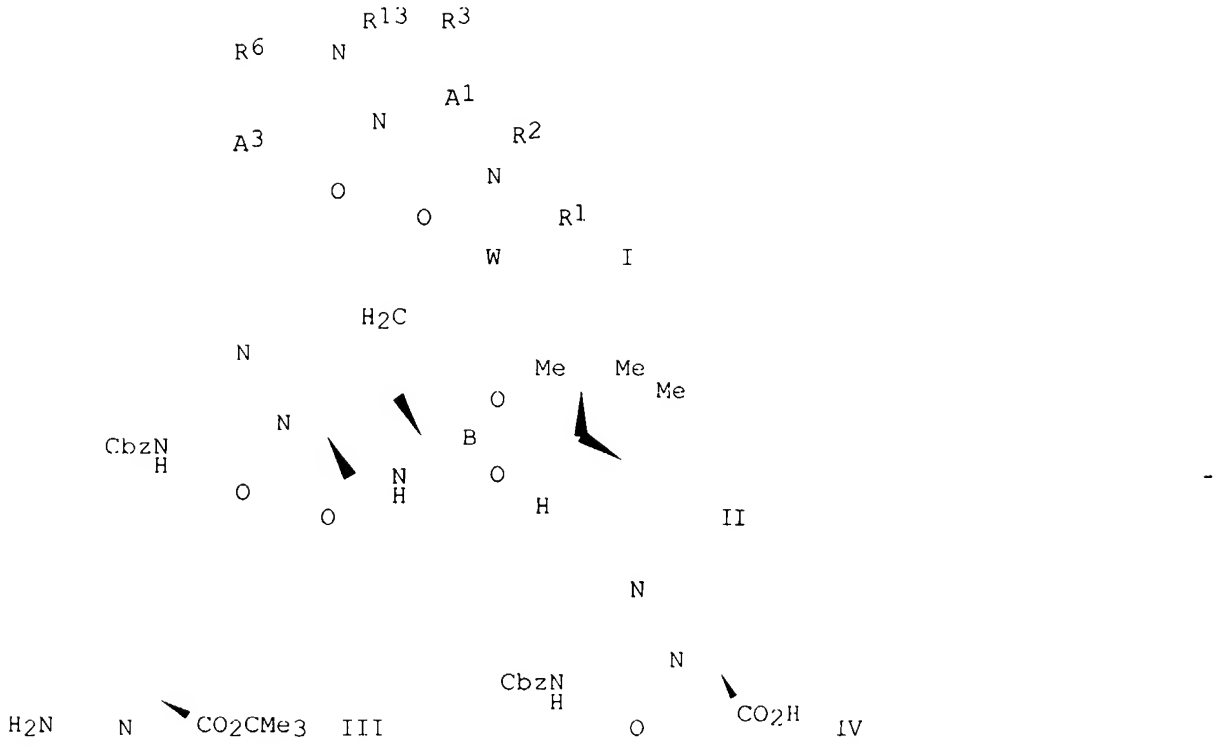
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 4 OF 17 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:465982 HCAPLUS
DOCUMENT NUMBER: 137:47213
TITLE: Preparation of fused pyrimidinones and benzodioxaborolidinylpropylaminopyrrolo[1,2-a]pyrimidines as inhibitors of hepatitis C ns3 protease for the treatment of hepatitis C and other viral diseases
INVENTOR(S): Glunz, Peter W.; Douty, Brent D.; Han, Wei
PATENT ASSIGNEE(S): Bristol-Myers Squibb Pharma Company, USA
SOURCE: PCT Int. Appl., 270 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002048116	A2	20020620	WO 2001-US47911	20011212
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002030763	A5	20020624	AU 2002-30763	20011212
US 2003064962	A1	20030403	US 2001-15304	20011212

PRIORITY APPLN. INFO.: US 2000-255290P P 20001213
WO 2001-US47911 W 20011212

OTHER SOURCE(S): MARPAT 137:47213
GI



AB Fused pyrimidinones I [A1 = (un)substituted CH2, CH2CH2, CH2CH2CH2, A2CH2, A2CH2CH2, CH2A2CH2; A2 = O, S, (un)substituted imino; A3 = H, R9CO, R9O, R9S, R9CONH, R9NHCO, etc.; W = (un)substituted **boronic** acid ester, QCOCO, QNHCOCO, QOCOCO, QNHCOCF2CO, COQ3, F3CCO, F3CCF2CO, OHC, amino acid residue; Q3 = (un)substituted aryl, heterocyclyl; R1 = H, F, (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl; R2 = H, alkyl; Q, R3, R9 = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, heterocyclyl; R6, R13 = H, (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, aralkyl, cycloalkylalkyl; R3R13 = (un)substituted carbocyclic ring, alkylidene] and particularly dioxaborolylpropylamino pyrrolopyriminecarboxamides such as II are prepd. as inhibitors of hepatitis C viral protein ns3 protease for the treatment of hepatitis C and other viral diseases. E.g., esterification of L-pyroglutamic acid with AcOCMe3 and HClO4, thionation with Lawesson's reagent, S-methylation with MeI, and amidation with NH4Cl gives nonracemic aminopyrrolinecarboxylate III. Treatment of III with di-Me 2-(methoxymethylene)malonate, hydrolysis of the Me ester moiety with LiOH, prepn. of the acyl azide with diphenylphosphoryl azide and Curtius rearrangement in the presence of PhCH2OH, and hydrolysis of the tert-Bu ester with CF3CO2H gives pyrrolo[1,2-a]pyrimidine IV. Coupling of IV with an .alpha.-allyl **aminomethylboronate** pinanediol ester gives II. I inhibit hepatitis C ns3 protease with IC50 values of <100 .mu.M. Pharmaceutical compns. contg. I are given.

IT **204765-53-7 438493-20-0**
RL: PRP (Properties)
(Unclaimed; prepn. of fused pyrimidinones and benzodioxaborolidinylpropylaminopyrrolo[1,2-a]pyrimidines as inhibitors of hepatitis C ns3 protease for the treatment of hepatitis C and other viral diseases)

IT **319010-09-8P**
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. of an assay substrate inhibitor for hepatitis C ns3 protease in the testing of fused pyrimidinone and benzodioxaborolidinylpropylaminop yrrolo[1,2-a]pyrimidine inhibitors of hepatitis C ns3 protease)

IT **99429-45-5P 274918-51-3P 319010-06-5P 319011-72-8P 319011-74-0P 319011-76-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of an assay substrate inhibitor for hepatitis C ns3 protease in the testing of fused pyrimidinone and benzodioxaborolidinylpropylaminop yrrolo[1,2-a]pyrimidine inhibitors of hepatitis C ns3 protease)

L47 ANSWER 5 OF 17 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:365340 HCAPLUS
DOCUMENT NUMBER: 137:93992
TITLE: Solid-Phase Synthesis and Biochemical Studies of O-Boranophosphopeptides and O-Dithiophosphopeptides
AUTHOR(S): Jenkins, Kenneth E.; Higson, Adrian P.; Seeberger, Peter H.; Caruthers, Marvin H.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO, 80309-0215, USA
SOURCE: Journal of the American Chemical Society (2002), 124(23), 6584-6593
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:93992

AB The authors present the solid-phase synthesis of two novel classes of phosphopeptide mimetics, O-boranophosphopeptides and O-dithiophosphopeptides, derivatized on tyrosine, serine, and threonine. The use of H-phosphonate and H-phosphonothioate monoesters contg. the base labile 9-fluorenemethyl protecting group was key to the synthesis of both phosphopeptide mimetics. O-Boranophosphopeptides were synthesized by condensing O-(9-fluorenemethyl)-H-phosphonate to the peptide hydroxylic component (Tyr, Ser or Thr) followed by oxidn. with BH3.cntdot.THF complex. Similarly, the synthesis of O-dithiophosphopeptides used the O-(9-fluorenemethyl)-H-phosphonothioate synthon and oxidn. with elemental sulfur. Base elimination of the 9-fluorenemethyl protecting group and cleavage from the solid support with concd. ammonium hydroxide afforded the boranophosphopeptide and dithiophosphopeptide target compds. Ac-Tyr-Ile-Ile-Pro-Leu-Pro-Gly-NH2, having either dithiophosphoryltyrosine or boranophosphoryltyrosine but no sequence specificity for Yersinia protein tyrosine phosphatase (PTP), was found to competitively inhibit this enzyme with KI values of 430 .+-. 50 and 670 .+-. 50 .mu.M, resp. In addn., both phosphopeptide analogs were resistant toward Yersinia PTP enzymic hydrolysis. Under conditions (pH 8.0) where the phosphopeptide was rapidly dephosphorylated, the boranophosphopeptide hydrolyzed slowly (t1/2 = 15 h) and the dithiophosphopeptide was completely stable over 24 h.

IT **14044-65-6**, Borane-tetrahydrofuran
RL: RCT (Reactant); RACT (Reactant or reagent)
(as a reactant in the solid-phase synthesis of O-boranophosphopeptides)

IT **441070-26-4P 441070-27-5P 441070-28-6P 441070-29-7P 441070-30-0P 441070-31-1P 442154-96-3P 442154-98-5P 442154-99-6P**
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(solid-phase synthesis of O-boranophosphopeptides and O-dithiophosphopeptides, their stability towards enzymic hydrolysis and their inhibition of protein tyrosine phosphatase)

REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 6 OF 17 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:119131 HCAPLUS
DOCUMENT NUMBER: 137:306551
TITLE: Hepatitis C Virus NS3 Protease Requires Its NS4A Cofactor Peptide for Optimal Binding of a **Boronic** Acid Inhibitor as Shown by NMR
AUTHOR(S): Archer, Sharon J.; Camac, Daniel M.; Wu, Zhongren J.; Farrow, Neil A.; Domaille, Peter J.; Wasserman, Zelda R.; Bukhtiyarova, Marina; Rizzo, Christopher; Jagannathan, Sharada; Mersinger, Lawrence J.; Kettner, Charles A.
CORPORATE SOURCE: DuPont Pharmaceuticals Company, Wilmington, DE, 19880, USA
SOURCE: Chemistry & Biology (2002), 9(1), 79-92
CODEN: CBOLE2; ISSN: 1074-5521
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB NMR spectroscopy was used to characterize the hepatitis C virus (HCV) NS3 protease in a complex with the 24 residue peptide cofactor from NS4A and a **boronic** acid inhibitor, Ac-Asp-Glu-Val-Val-Pro-boroAlg-OH. Secondary-structure information, NOE constraints between protease and cofactor, and hydrogen-deuterium exchange rates revealed that the cofactor was an integral strand in the N-terminal .beta.-sheet of the complex as obsd. in X-ray crystal structures. Based upon chem.-shift perturbations, inhibitor-protein NOEs, and the protonation state of the catalytic histidine, the **boronic** acid inhibitor was bound in the substrate binding site as a transition state mimic. In the absence of cofactor, the inhibitor had a lower affinity for the protease. Although the inhibitor binds in the same location, differences were obsd. at the catalytic site of the protease.
IT **204765-53-7D**, complexes with NS3 protease **319010-17-8D**, complexes with NS3 protease
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(hepatitis C virus NS3 protease requires NS4A cofactor peptide for optimal binding of **boronic** acid inhibitor as shown by NMR)
REFERENCE COUNT: 68 THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 7 OF 17 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:46816 HCAPLUS
DOCUMENT NUMBER: 137:263279
TITLE: nitrogen to carbon SPPS using 9-fluorenylmethyl esters or phase transfer catalyst salts: development and application to the synthesis of peptidic amino **boronates** and phosphonates
AUTHOR(S): Merette, Sandrine A. M.; Burd, Andrew P.; Teakle, Ngari; Scully, Michael F.; Kakkar, Vijay V.; Deadman, John J.
CORPORATE SOURCE: Thrombosis Research Institute, London, SW3 6LR, UK
SOURCE: Innovation and Perspectives in Solid Phase Synthesis & Combinatorial Libraries: Peptides, Proteins and Nucleic Acids--Small Molecule Organic Chemistry Diversity, Collected Papers, International Symposium, 6th, York, United Kingdom, Aug. 31-Sept. 4, 1999 (2001), Meeting Date 1999, 51-56. Editor(s): Epton, Roger. Mayflower Scientific Ltd.: Kingswinford, UK.
CODEN: 69CEGV; ISBN: 0-9515735-3-5
DOCUMENT TYPE: Conference
LANGUAGE: English
AB A symposium report. A novel strategy of loading the resin with an amino acid as its phase transfer catalyst (PTC) salt is presented. The PTC

salts and 9-fluorenylmethyl esters coupled quant. to the p-nitrophenyl carbonate Wang resin in NMP. The method was applied to the synthesis of peptidic amino phosphonates and **boronates**.

IT **463326-11-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of peptidic amino **boronates** and phosphonates by nitrogen to carbonyl solid phase peptide synthesis)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 8 OF 17 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:923642 HCAPLUS
DOCUMENT NUMBER: 136:74618
TITLE: Prodrug compounds with isoleucine
INVENTOR(S): Pickford, Lesley B.; Gangwar, Sanjeev; Lobl, Thomas J.; Nieder, Matthew H.; Yarranton, Geoffrey T.
PATENT ASSIGNEE(S): Corixa Corporation, USA
SOURCE: PCT Int. Appl., 107 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001095943	A2	20011220	WO 2001-US18857	20010611
WO 2001095943	A3	20020829		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1294404	A2	20030326	EP 2001-944442	20010611
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				

PRIORITY APPLN. INFO.: US 2000-211686P P 20000614
WO 2001-US18857 W 20010611

OTHER SOURCE(S): MARPAT 136:74618

AB The compds. of the invention are modified forms of therapeutic agents. A typical prodrug compd. of the invention comprises a therapeutic agent, an oligopeptide having an isoleucine residue, a stabilizing group and, optionally, a linker group. The prodrug is cleavable by an enzyme assocd. with the target cell. Methods of making and using the compds. are also disclosed.

IT **123884-00-4**, Dolastatin 15
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(prodrug compds. with isoleucine)

IT **14047-29-1**, 4-Carboxyphenyl **boronic** acid
RL: MOA (Modifier or additive use); USES (Uses)
(stabilizing agent; prodrug compds. with isoleucine)

L47 ANSWER 9 OF 17 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:661423 HCAPLUS
DOCUMENT NUMBER: 135:227016
TITLE: Preparation of N-[1-(4,6-methano-1,3,2-benzodioxaborol-2-yl)-3-butenyl]pyrrolo[1,2-a]pyrazine-6-carboxamides as Hepatitis C virus NS3 protease inhibitors
INVENTOR(S): Zhang, Xiaojun; Han, Wei

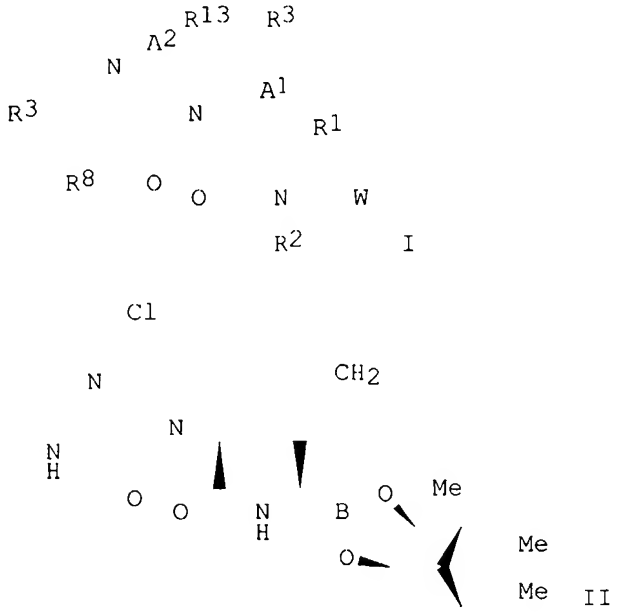
PATENT ASSIGNEE(S): Dupont Pharmaceuticals Company, USA
SOURCE: PCT Int. Appl., 191 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001064678	A2	20010907	WO 2001-US6269	20010228
WO 2001064678	A3	20020307		
W: AT, AU, BR, CA, CH, CZ, DE, DK, EE, ES, FI, GB, HU, IL, IN, JP, KR, LT, LU, LV, MX, NO, NZ, PL, PT, RO, SE, SG, SI, SK, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
US 2002065248	A1	20020530	US 2001-795410	20010228
EP 1261611	A2	20021204	EP 2001-918260	20010228
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003525294	T2	20030826	JP 2001-564175	20010228

PRIORITY APPLN. INFO.: US 2000-185618P P 20000229
WO 2001-US6269 W 20010228

OTHER SOURCE(S): MARPAT 135:227016

GI



AB The present invention relates to the prepn. and use of the title compds. (I) [wherein A1 = methylene, ethylene, or propylene; A2 = N or CR6; A3 = amino acid or di- or tripeptide residue, SOR9, SO2R9, COR9, CO2R9, CONHR9, etc.; R9 = H or (un)substituted (cyclo)alkyl, aryl, or heterocyclyl; W = BO2H2, COCOQ, COCONHQ, COCOOQ, COCF2CONHQ, COCF3, COCF2CF3, CHO, amino acid residue, or di- or tripeptide residue; Q = (un)substituted alkyl,- alkenyl, alkynyl, amino acid residue, di- or tripeptide residue, etc.; R1 = H, F, or (un)substituted (cyclo)alkyl, alkenyl, alkynyl, or aryl; R2 and R8 = independently H, (cyclo)alkyl, alkenyl, or alkynyl; R3 = R4, OR4, SR4, or (un)substituted amino; R4 = (un)substituted (cyclo)alkyl, alkenyl,

alkynyl, aryl, or heterocyclyl; R13 = H or alkyl; stereoisomeric forms, stereoisomeric mixts., or pharmaceutically acceptable salt forms thereof] as inhibitors of Hepatitis C virus (HCV) NS3 protease. For example, esterification of Boc-Glu-OMe with EtSH, followed by redn. to the aldehyde using SiEt3H and cyclization in MeOH, gave the 5-methoxy-2-pyrrolidinecarboxylate intermediate. Conversion to the 5-cyano pyroglutamate, deprotection, and cycloaddn. with oxalyl chloride afforded the pyrrolo[1,2-a]pyrazine-6-oxoacetate. Addn. of 4-methoxybenzylamine, followed by treatment with LiOH and amidation with Alg-boro-C10H16O2, gave II. A no. of compds. I inhibited HCV NS3 protease with Ki values of .ltoreq. 60 .mu.M. The invention also relates to pharmaceutical compns. and diagnostic kits comprising I, and methods of using I for treating viral infection or as an assay std. or reagent.

IT **99429-45-5P 274918-51-3P 319010-06-5P**
319011-72-8P 319011-74-0P 319011-76-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prepn. of methanobenzodioxaborolylbutenyl pyrrolopyrazinecarboxamide HCV NS3 protease inhibitors by cyclization of glutamates to pyrrolidines, cycloaddn. with oxalyl chloride, and amidation with boroles)

IT **359028-78-7P 359028-79-8P 359028-80-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of methanobenzodioxaborolylbutenyl pyrrolopyrazinecarboxamide HCV NS3 protease inhibitors by cyclization of glutamates to pyrrolidines, cycloaddn. with oxalyl chloride, and amidation with boroles)

IT **319010-09-8P**
RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(protease inhibitor; prepn. of methanobenzodioxaborolylbutenyl pyrrolopyrazinecarboxamide HCV NS3 protease inhibitors by cyclization of glutamates to pyrrolidines, cycloaddn. with oxalyl chloride, and amidation with boroles)

IT **98-80-6, Phenylboronic** acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; prepn. of methanobenzodioxaborolylbutenyl pyrrolopyrazinecarboxamide HCV NS3 protease inhibitors by cyclization of glutamates to pyrrolidines, cycloaddn. with oxalyl chloride, and amidation with boroles)

L47 ANSWER 10 OF 17 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:616788 HCAPLUS
DOCUMENT NUMBER: 135:358140
TITLE: The development of highly efficient onium-type peptide coupling reagents based upon rational molecular design
AUTHOR(S): Li, P.; Xu, J. C.
CORPORATE SOURCE: Laboratory of Medicinal Chemistry, National Cancer Institute, National Institute of Health, Frederick, MD, 21702, USA
SOURCE: Journal of Peptide Research (2001), 58(2), 129-139
CODEN: JPERFA; ISSN: 1397-002X
PUBLISHER: Munksgaard International Publishers Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Novel and highly efficient immonium-, pyridinium- and thiazolium-type peptide coupling reagents, such as BOMI, BDMP, BPMP, BEP, FEP, BEPH, FEPH and BEMT, were developed by rational modifying of the mol. structures of commonly used uronium-type reagents. The high efficiency of these onium salts has been evaluated and proven by model reaction tests and the successful synthesis of various oligopeptides and biol. active peptides,

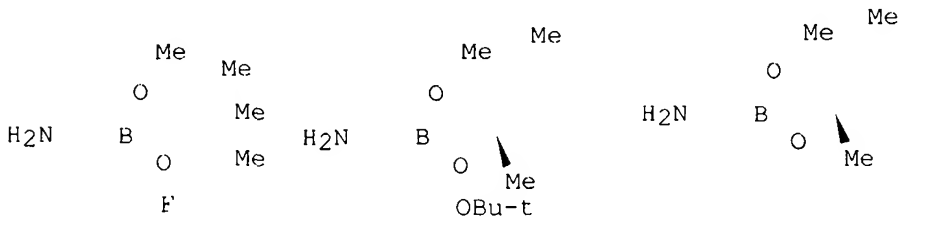
both in soln. and in the solid-phase, for example Leu-enkephalin, the pentapeptide moiety of Dolastatin 15 and the immunosuppressive undecapeptide cyclosporin O. Based upon these results, the relationship between the mol. structure and the capability of onium-type peptide coupling reagents was studied. A preliminary guideline for the mol. design of onium-type coupling reagents was developed.

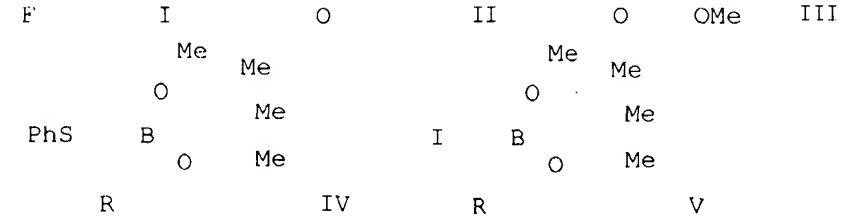
IT **368-39-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. and use of peptide coupling reagents based on onium-type structures)

IT **215393-04-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and use of peptide coupling reagents based on onium-type structures)

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 11 OF 17 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:604212 HCAPLUS
DOCUMENT NUMBER: 135:331665
TITLE: Synthesis of **Boronic** Acid Analogues of .alpha.-Amino Acids by Introducing Side Chains as Electrophiles
AUTHOR(S): Jagannathan, Sharada; Forsyth, Timothy P.; Kettner, Charles A.
CORPORATE SOURCE: Chemical and Physical Sciences, Dupont Pharmaceuticals Company, Wilmington, DE, 19880-0500, USA
SOURCE: Journal of Organic Chemistry (2001), 66(19), 6375-6380
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:331665
GI





AB This work describes the synthesis of .alpha.-**aminoboronic** acids and their incorporation into peptides as inhibitors of serine proteases. For example, .alpha.-**aminoboronic** acids I-III were prepd. II and III are **boronic** acid analogs of aspartic acid and glutamic acid with the side chain carboxylate protected as a tert-Bu or a Me ester,

resp. The key step of the synthesis was that the side chains of the .alpha.-**aminoboronic** acids were introduced as electrophiles (this is particularly advantageous for side chains which are prone to elimination or unwanted enolate formation). For example, BrCH2CHF2, BrCH2CO2Bu-t, and H2C:CHCO2Me were allowed to react with the stabilized anion of (phenylthio)methane **boronate** IV (R = H) to give the substituted **boronate** intermediates IV (R = CH2CHF2, CH2CO2Bu-t, CH2CH2CO2Me). Next, these intermediates were converted to the corresponding sulfonium ion by treatment with Me iodide and then converted to the iodide V (R as in IV). The iodo moiety in V was converted to the amine by conventional methods (the synthesis of II and III included a transesterification step with (+)-pinanediol ester).

IT **370103-58-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of **boronic** acid analogs of amino acids by introducing side chains as electrophiles)

IT **370095-79-7P 370095-80-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of peptides contg. **boronic** acid analogs of amino acids and the biol. activity of these peptides as hepatitis C protease inhibitors)

IT **319012-18-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
*(prepn. of peptides contg. **boronic** acid analogs of amino* acids and the biol. activity of these peptides as hepatitis C protease inhibitors)

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 12 OF 17 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2001:31525 HCAPLUS
DOCUMENT NUMBER: 134:101193
TITLE: Preparation of peptide **boronic** acid inhibitors of hepatitis C virus protease
INVENTOR(S): Kettner, Charles A.; Jagannathan, Sharada; Forsyth, Timothy Patrick
PATENT ASSIGNEE(S): Du Pont Pharmaceuticals Company, USA
SOURCE: PCT Int. Appl., 258 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001002424	A2	20010111	WO 2000-US18655	20000707
WO 2001002424	A3	20010719		
W: AU, BR, CA, CN, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, TR, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 2000057888	A5	20010122	AU 2000-57888	20000707
EP 1196436	A2	20020417	EP 2000-943413	20000707
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				

PRIORITY APPLN. INFO.: US 1999-142561P P 19990707
WO 2000-US18655 W 20000707
OTHER SOURCE(S): MARPAT 134:101193
AB .alpha.-**Aminoboronic** acids and corresponding peptide analogs

R3-A-NR2CHR1BY1Y2 [Y1, Y2 = OH, F, an amino group, alkoxy or BY1Y2 is a cyclic **boron** ester, amide or amide-ester; R1 = CH:CH2, CH2CH:CH2, CH:CHCH3, C.tplbond.CH, C.tplbond.CCH3, CH2C.tplbond.CH, cyclopropyl, cyclopropylmethyl, cyclobutyl, cyclobutylmethyl, mercaptoalkyl, alkyldithioalkyl, etc.; A is a bond, a natural or unnatural amino acid residue, or a peptide residue comprising 2-10 amino acids; R2 = H, alkyl, aryl, arylalkyl, cycloalkyl; R3 = H, alkanoyl, alkyl, alkenyl, alkynyl, aryl, carbalkoxy, alkylsulfinyl, alkylsulfonyl, carbamoyl, etc.] were prepd. for the treatment of hepatitis C viral infections. Thus, Boc-Asp(OBu-t)-Glu(OBu-t)-Val-Val-Pro-boroCpa-OH pinanediol ester (Boc = tert-butoxycarbonyl, boroCpa is L-2-amino-3-**cyclopropylboronic** acid residue) was prepd. by std. methods of peptide coupling in soln. Enzyme assays, dosages and formulations are discussed.

IT **98-80-6, Phenylboronic** acid **5419-55-6,** Triisopropyl borate **94242-85-0 319012-18-5**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of peptide **boronic** acid inhibitors of hepatitis C virus protease)

IT **99429-45-5P 274918-51-3P 319010-02-1P 319010-04-3P 319010-06-5P 319010-09-8P 319010-11-2P 319010-13-4P 319010-15-6P 319010-17-8P 319010-19-0P 319010-21-4P 319010-23-6P 319010-25-8P 319010-27-0P 319010-29-2P 319010-42-9P 319010-44-1P 319010-46-3P 319010-48-5P 319010-50-9P 319010-52-1P 319010-54-3P 319010-56-5P 319010-58-7P 319010-60-1P 319010-62-3P 319010-64-5P 319010-66-7P 319010-68-9P 319010-70-3P 319010-74-7P 319010-80-5P 319010-82-7P 319010-84-9P 319010-86-1P 319010-88-3P 319010-90-7P 319010-92-9P 319010-94-1P 319010-96-3P 319011-72-8P 319011-74-0P 319011-76-2P 319011-78-4P 319011-91-1P 319011-93-3P 319012-16-3P 319012-22-1P 319012-24-3P 319012-26-5P 319012-28-7P 319012-30-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of peptide **boronic** acid inhibitors of hepatitis C virus protease)

IT **319007-13-1P 319007-15-3P 319007-17-5P 319007-20-0P 319007-22-2P 319007-24-4P 319007-26-6P 319007-28-8P 319007-30-2P 319007-32-4P 319007-34-6P 319007-36-8P 319007-38-0P 319007-40-4P 319007-42-6P 319007-44-8P 319007-46-0P 319007-48-2P 319007-50-6P 319007-52-8P 319007-54-0P 319007-56-2P 319007-58-4P 319007-60-8P 319007-62-0P 319007-64-2P 319007-66-4P 319007-68-6P 319007-70-0P 319007-72-2P 319007-74-4P 319007-76-6P 319007-78-8P 319007-80-2P 319007-82-4P 319007-84-6P 319007-86-8P 319007-88-0P 319007-90-4P 319007-92-6P 319007-94-8P 319007-96-0P 319007-98-2P 319008-00-9P 319008-02-1P 319008-04-3P 319008-06-5P 319008-08-7P 319008-10-1P 319008-12-3P 319008-14-5P 319008-16-7P 319008-18-9P 319008-20-3P 319008-22-5P 319008-24-7P 319008-26-9P 319008-28-1P 319008-30-5P 319008-32-7P 319428-29-0P**
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptide **boronic** acid inhibitors of hepatitis C virus protease)

L47 ANSWER 13 OF 17 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:607748 HCAPLUS
DOCUMENT NUMBER: 133:335259
TITLE: 1-**Aminocyclopropaneboronic** Acid: Synthesis and Incorporation into an Inhibitor of Hepatitis C Virus NS3 Protease
AUTHOR(S): Priestley, E. Scott; Decicco, Carl P.
CORPORATE SOURCE: Department of Chemical and Physical Sciences, DuPont Pharmaceuticals Company, Wilmington, DE, 19880, USA
SOURCE: *Organic Letters (2000), 2(20), 3095-3097*
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 133:335259
AB The previously unreported .alpha.,.alpha.-disubstituted 1-**aminoboronate** esters have potential utility in peptidomimetic design, particularly against serine protease targets. A concise synthesis of 1-**aminocyclopropaneboronate** pinanediol ester is reported, and a peptidyl deriv. has modest affinity (Ki = 1.6 .mu.M) for hepatitis C NS3 protease. Analogs with iso-Pr and cyclohexyl in place of cyclopropyl were also prepd. and tested.
IT **274918-51-3**, *Boc-Asp(O-t-Bu)-Glu(O-t-Bu)-Val-Val-Pro-OH*
RL: RCT (Reactant); RACT (Reactant or reagent)
(coupling with .alpha.,.alpha.-disubstituted 1-**aminoboronate** esters)
IT **5419-55-6**, Triisopropyl borate
RL: RCT (Reactant); RACT (Reactant or reagent)
(for prepn. of .alpha.,.alpha.-disubstituted 1-**aminoboronate** esters)
IT **303191-80-2P 303191-81-3P 303191-82-4P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and activity as inhibitor of hepatitis C NS3 protease)
IT **303191-77-7P 303191-78-8P 303191-79-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and deprotection of)
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 14 OF 17 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:255214 HCAPLUS
DOCUMENT NUMBER: 133:74283
TITLE: Total synthesis of Cyclosporin O both in solution and in the solid phase using novel thiazolium-, immonium-, and pyridinium-type coupling reagents: BEMT, BDMP, and BEP
AUTHOR(S): Li, Peng; Xu, Jie Cheng
CORPORATE SOURCE: Shanghai Institute of Organic Chemistry, Chinese Academy of Sciences, Shanghai, 200032, Peop. Rep. China
SOURCE: Journal of Organic Chemistry (2000), 65(10), 2951-2958
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Cyclosporin O (CsO), an extensively N-methylated immunosuppressive cyclic undecapeptide, was synthesized in 20-23% overall yield via 4 + 7 segment

condensation and cyclization by the combined utilization of novel thiazolium- and immonium-type peptide coupling reagents, 2-bromo-3-ethyl-4-Me thiazolium tetrafluoroborate (BEMT) and 5-(1H-benzotriazol-1-yloxy)-3,4-dihydro-1-Me 2H-pyrrolium hexachloroantimonate (BDMP), as well as 2-bromo-1-Et pyridinium tetrafluoroborate (BEP). BEMT and BEP (proven to be very efficient for the coupling of peptide segments contg. N-alkylated amino acid residues with respect to the fast reaction time, low racemization, and high yields) were used to construct hindered amide bonds in CsO with the addn. of HOAt, whereas the most efficient HOBt-derived immonium type reagent, BDMP, was used to perform the coupling of coded amino acids in CsO. Thus, the highly hindered protected CsO8-11 tetrapeptide, Fmoc-D-Ala-MeLeu-MeLeu-MeVal-OH, was successfully synthesized using BEMT in 65% yield, and the CsO1-7 heptapeptide, Fmoc-MeLeu-Nva-Sar-MeLeu-Val-MeLeu-Ala-OCH2Ph, was obtained in 52-55% yield by the rationally combined utilization of BDMP, BEMT and BEP. The synthesis of the linear undecapeptide, Fmoc-D-Ala-MeLeu-MeLeu-MeVal-MeLeu-Nva-Sar-MeLeu-Val-MeLeu-Ala-OH, of CsO in the solid-phase using BEMT and BEP was accomplished for the further evaluation of the effectiveness of these reagents.

IT **368-39-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of novel peptide coupling agents for use in total synthesis of cyclosporin O)

IT **270085-21-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of peptides contg. N-methylamino acids with BEMT and BEP as peptide coupling agents)

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 15 OF 17 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:626226 HCAPLUS
DOCUMENT NUMBER: 131:241986
TITLE: Methods for identifying inducers and inhibitors of proteolytic antibodies, compositions and their uses
INVENTOR(S): Paul, Sudhir; Gololobov, Gennady; Smith, Larry
PATENT ASSIGNEE(S): University of Nebraska Board of Regents, USA
SOURCE: PCT Int. Appl., 158 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9948925	A1	19990930	WO 1999-US6325	19990323
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6235714	B1	20010522	US 1998-46373	19980323
CA 2324340	AA	19990930	CA 1999-2324340	19990323
AU 9931113	A1	19991018	AU 1999-31113	19990323
AU 760648	B2	20030522		
BR 9909011	A	20001128	BR 1999-9011	19990323
EP 1064308	A1	20010103	EP 1999-912835	19990323
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

IE, FI
JP 2002507627 T2 20020312 JP 2000-537907 19990323
PRIORITY APPLN. INFO.: US 1998-46373 A 19980323
WO 1999-US6325 W 19990323

AB Disclosed herein are covalently reactive antigen analogs comprising epitope of tumor necrosis factor, EGF receptor, interleukin 1, gp120, gp160, gag, pol, hepatitis B surface antigen, bacterial exotoxin, EGF, TGF.alpha., p53, prostate-specific antigen, carcinoembryonic antigen, prolactin, human chorionic gonadotropin, c-myc, c-fos, c-jun, HER-2, prolactin receptor, steroid receptor or interleukin 4.. The antigens of the invention may be used to stimulate prodn. of catalytic antibodies specific for predetd. antigens assocd. with particular medical disorders. The antigen analogs may also be used to permanently inactivate endogenously produced catalytic antibodies produced in certain autoimmune diseases as well as in certain lymphoproliferative disorders. The invention also provides methods for identifying, isolating and prodn. of catalytic antibodies with therapeutic value.

IT **244245-89-4P**
RL: BPN (Biosynthetic preparation); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(covalently reactive antigen analogs for inhibition or prodn. of proteolytic antibodies and for treating autoimmune diseases, cancer, infection, inflammation and lymphoproliferative disorders)

IT **13780-71-7D**, **Boronic** acid, peptide esters
RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(covalently reactive antigen analogs for inhibition or prodn. of proteolytic antibodies and for treating autoimmune diseases, cancer, infection, inflammation and lymphoproliferative disorders)

IT **244279-26-3**
RL: PRP (Properties)
(unclaimed sequence; methods for identifying inducers and inhibitors of proteolytic antibodies, compns. and their uses)

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L47 ANSWER 16 OF 17 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:618094 HCAPLUS
DOCUMENT NUMBER: 127:263058
TITLE: Preparation of novel amide bond-containing thiol derivatives as endothelin converting enzyme inhibitors
INVENTOR(S): Deprez, Pierre; Dumas, Jacques; Fournie-Zaluski, Marie-Claude; Guillaume, Jacques; Roques, Bernard Pierre
PATENT ASSIGNEE(S): Roussel-UCLAF, Fr.; Institut National de la Sante et de la Recherche Medicale (INSERM); Deprez, Pierre; Dumas, Jacques; Fournie-Zaluski, Marie-Claude; Guillaume, Jacques; Roques, Bernard Pierre
SOURCE: PCT Int. Appl., 75 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9732874	A1	19970912	WO 1997-FR367	19970303
W: AU, BR, CA, CN, HU, IL, JP, KR, MX, NO, PL, RU, TR, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
FR 2745571	A1	19970905	FR 1996-2672	19960304
FR 2745571	B1	19980619		
CA 2248187	AA	19970912	CA 1997-2248187	19970303

AU 9719306	A1	19970922	AU 1997-19306	19970303
AU 724686	B2	20000928		
EP 888341	A1	19990107	EP 1997-907157	19970303
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
CN 1218467	A	19990602	CN 1997-194380	19970303
BR 9707931	A	19990727	BR 1997-7931	19970303
JP 2000507220	T2	20000613	JP 1997-531511	19970303
RU 2203661	C2	20030510	RU 1998-118049	19970303
NO 9804047	A	19981103	NO 1998-4047	19980903
US 6136842	A	20001024	US 1999-142286	19990112
PRIORITY APPLN. INFO.:			FR 1996-2672 A	19960304
			WO 1997-FR367 W	19970303

OTHER SOURCE(S): MARPAT 127:263058

AB Thiol derivs. HS(CH2)nCH(CH2R1)CONHCHR2A (n = 0, 1; R1 = substituted Ph or biphenyl; R2 = H, substituted benzyl, phenylthiomethyl, or indolylmethyl; A = carboxy or a salt, ester, or amide, tetrazolyl, or substituted alkyl) were prepd. as endothelin converting enzyme (ECE) inhibitors. Thus, N-[3-(3-bromophenyl)-2-(mercaptomethyl)-1-oxopropyl]-L-tryptophan was prepd. via a 6-step procedure starting from Me 2-(dimethylamino)propanoate, 3-bromobenzyl bromide, thioacetic acid, and L-tryptophan. The product was assayed for ECE inhibitor activity (CI50 = 20 nM).

IT **196302-81-5P**
RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of novel amide bond-contg. thiol derivs. as endothelin converting enzyme inhibitors)

IT **98-80-6, Phenylboronic** acid **5720-07-0**, 4-**Methoxybenzeneboronic** acid **6165-68-0**, 2-**Thiopheneboronic** acid **151780-69-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of novel amide bond-contg. thiol derivs. as endothelin converting enzyme inhibitors)

L47 ANSWER 17 OF 17 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:457230 HCAPLUS
DOCUMENT NUMBER: 127:62846
TITLE: Membranes and membrane DNA/RNA sensors
INVENTOR(S): *Schalkhammer, Thomas; Pittner, Fritz*
PATENT ASSIGNEE(S): Schalkhammer, Thomas, Austria; Pittner, Fritz
SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9720203	A1	19970605	WO 1996-AT230	19961121
W: US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AT 9501943	A	19970415	AT 1995-1943	19951128
AT 403215	B	19971229		
AT 9600485	A	19971115	AT 1996-485	19960314
PRIORITY APPLN. INFO.:			AT 1995-1943	19951128
			AT 1996-485	19960314

AB The invention concerns a novel highly sensitive membrane sensor which, in particular, uses a novel membrane structure. *The interaction between* lipid layers is reinforced by using the reaction between **organoboron** compds., and/or stable lipids of the given general formulas are used. This novel sensor is designed as a hybridization-controlled membrane channel biosensor. The membrane channel

biosensor uses the bonding of DNA and RNA to an immobilized capture oligonucleotide to control a membrane channel. Examples are given of the prepn. of sensors for herpes virus, HIV-1, HIV-2, etc.

IT **7440-42-8D, Boron**, org. compds., uses
RL: ARG (Analytical reagent use); DEV (Device component use); ANST (Analytical study); USES (Uses)
(membranes and membrane channel biosensors)

IT **191600-26-7**
RL: BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(membranes and membrane channel biosensors)

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L48             1 SEA FILE=REGISTRY ABB=ON  PLU=ON  PHENYLPROPYLBORON/BI
L49             9 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L48 OR PHENYLPROPYLBORON? OR
                  PHENYL?(2A)PROPYL?(2A)BORON?


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=> d ibib abs hitrn 149 1-9

L49  ANSWER 1 OF 9  HCAPLUS  COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:         2002:555500  HCAPLUS
DOCUMENT NUMBER:          137:109373
TITLE:                    Preparation of serine protease inhibitors comprising a
                          non-peptide boronate or other hydrogen-bond acceptor
INVENTOR(S):              Deadman, John Joseph; Spencer, John; Greenidge,
                          Paulette Angela; Goodwin, Christopher Andrew; Kakkar,
                          Vijay Vir; Scully, Michael Finbarr
PATENT ASSIGNEE(S):       Trigen Limited, UK
SOURCE:                   PCT Int. Appl., 117 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
     ---------------   ----  --------       ---------------  --------
     WO 2002057273      A1   20020725       WO 2002-GB224    20020118
     WO 2002057273      C2   20021128
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
             TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
PRIORITY APPLN. INFO.:                    GB 2001-1537     A  20010120
                                          US 2001-267172P  P  20010206
OTHER SOURCE(S):          MARPAT 137:109373
AB   X-Ar-LJ (I; e.g. isothiouronium salts 2-(2-((carbamimidoylthio)methyl)phen
     yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane hydrobromide and 3-nitrobenzyl
     carbamimidothioate hydrobromide) are useful as protease inhibitors.  In I,
     Ar is a ring or ring system, for example a benzene ring, and may be
     substituted by one or more moieties in addn. to X and LJ; X is a
     functional group which is a H bond acceptor, e.g. a nitro or boronate
     group BY1Y2; L is a linker, most preferably (CR5R6)-S-; J is a moiety
     contg. a basic N atom but not contg. an amino acid residue, preferably
     amidino, guanidino, amino, carboxamido, hydroxylamino, or imidazolyl, or
     an N-substituted analog thereof.  Enzyme inhibition activities for some of
     the claimed compds. for up to 6 enzymes (plasmin, thrombin, trypsin,
     factor IX, factor X, urokinase) are reported.  Several methods of prepn.
     are claimed and 31 prepns. are included.
REFERENCE COUNT:          10    THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS
                                RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49  ANSWER 2 OF 9  HCAPLUS  COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:         2002:163800  HCAPLUS
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DOCUMENT NUMBER: 136:219519
TITLE: Phenyl boron-based compounds as anion receptors for nonaqueous battery electrolytes
INVENTOR(S): Lee, Hung Sui; Yang, Xiao-qing; McBreen, James; Sun, Xuehui
PATENT ASSIGNEE(S): Brookhaven Science Associates, Llc, USA
SOURCE: U.S., 15 pp., Cont.-in-part of U. S. 6,022,643.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6352798	B1	20020305	US 2000-492569	20000127
US 6022643	A	20000208	US 1997-986846	19971208

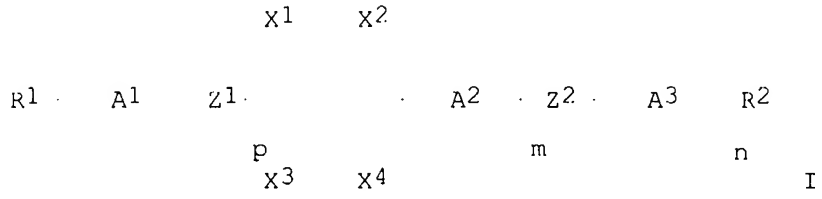
PRIORITY APPLN. INFO.: US 1997-986846 A2 19971208
OTHER SOURCE(S): MARPAT 136:219519
AB Novel fluorinated boronate-based compds. which act as anion receptors in nonaq. battery electrolytes are provided. When added to nonaq. battery electrolytes, the fluorinated boronate-based compds. of the invention enhance ionic cond. and cation transference no. of nonaq. electrolytes. The fluorinated boronate-based anion receptors include different fluorinated alkyl and aryl groups.
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:117111 HCAPLUS
DOCUMENT NUMBER: 137:140296
TITLE: Cross-coupling reactions of primary alkylboronic acids with aryl triflates and aryl halides
AUTHOR(S): Molander, Gary A.; Yun, Chang-Soo
CORPORATE SOURCE: Roy and Diana Vagelos Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, PA, 19104-6323, USA
SOURCE: Tetrahedron (2002), 58(8), 1465-1470
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 137:140296
AB The cross-coupling reactions of primary alkylboronic acids with aryl triflates and aryl halides was successfully achieved using PdCl2(dppf).cntdot.CH2Cl2 in the presence of K carbonate to provide the corresponding Suzuki coupled products in high yields.
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:851205 HCAPLUS
DOCUMENT NUMBER: 134:29199
TITLE: Method for preparation of biaryl derivatives by coupling reaction on arylboronic acids
INVENTOR(S): Goto, Yasuyuki; Nohgami, Masaki; Kobayashi, Katsuhiko
PATENT ASSIGNEE(S): Chisso Corp., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2000336045	A2	20001205	JP 1999-148564	19990527

PRIORITY APPLN. INFO.: JP 1999-148564 19990527
OTHER SOURCE(S): CASREACT 134:29199; MARPAT 134:29199
GI



AB The title compds. [I; R1 = F, Cl, H, (un)substituted C1-12 alkyl, alkoxy, or alkenyl optionally getting .gtoreq.1 CH2 groups replaced independently with O, S, CO, CO2, O2C, or OCO2 provided that O atoms are not directly bonded to each other; R2 = H, (un)substituted C1-12 alkyl, alkoxy, or alkenyl, cyano, thiocyanato, F, Cl; Z1, Z2 = CO2, O2C, CH2O, OCH2, CH2CH2, (CH2)4, CH:CHCH2CH2, CH2CH2CH:CH, CH:CH, C.tplbond.C, single bond; X1 - X4 = group listed in R1, cyano, thiocyanato, F, Cl; ring A, A2, or A3 = (un)substituted trans-1,4-cyclohexylene optionally getting nonadjacent .gtoreq.1 CH2 groups replaced with O or S, 1,4-phenylene, 1,4-cyclohexenylene, 1,4-bicyclo[2.2.2]octylene, piperidine-1,4-diyl, naphthalene-2,6-diyl, decahydronaphthalene-2,6-diyl, or 1,2,3,4-tetrahydronaphthalene-2,6-diyl optionally getting 1 or 2 CH2 groups replaced independently with O or S; p, m, n = 0, 1,2] are prepd. by coupling of arom. boronic acids (II; R1, ring A1, X1 - X4, p = same as above; R3, R4 = H, Me, Et, n-Pr, i-Pr) with aryl halides, heteroaryl halides, aryl fluoroalkanesulfonates, or heteroaryl fluoroalkanesulfonates (III; ring A2 or A3, Z2, R2, m, n = same as above; Y = Cl, Br, iodo, toluenesulfonyloxy, methanesulfonyloxy, CF3SO3) in the presence of palladium metal catalyst if necessary carried on a support, ligand selected from phosphins, diketones, or tertiary amines, base, and phase transfer catalyst. This process efficiently gives biaryl derivs., in particular having cyano, carbonyl, or hydroxy group on the arom. ring or polycyclic compds. having .gtoreq.3 rings in an industrial scale without increasing the use of catalyst. These compds. are useful as drugs, agrochems., or their intermediates, or as liq. crystal materials. Thus, 25.0 g 4-[4-(trans-4-**propylcyclohexyl**)**phenyl**] **boronic** acid and 15.0 g 2-chloro-5-ethylpyrimidine were dissolved in 50 mL PhMe and 20 mL 50% Et alc., followed by adding 27.6 g K2CO3, 21.28 mg 5% Pd-C, and 9.67 g Bu4NBr, and the resulting mixt. was refluxed for 6 h to give 80.0% 5-ethyl-2-[4-(4-trans-4-propylcyclohexyl)phenyl]pyrimidine, which showed CN and NI liq. crystal phase at 109.0 and 186.5.degree., resp.

L49 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2000:692807 HCAPLUS
DOCUMENT NUMBER: 134:131271
TITLE: Convenient route for the synthesis of 4-pentyl-(4'-propyl)trans-biscyclohexylbiphenyl under ultrasound
AUTHOR(S): Chen, Xin-Bing; An, Zhong-Wei; Liu, Qian-Feng; Gan, Yun-Qing
CORPORATE SOURCE: R &D Center of Liquid Crystal, Xian Modern Chemistry Research Institute, Xian, 710065, Peop. Rep. China
SOURCE: Hecheng Huaxue (2000), 8(4), 291-293

CODEN: HEHUE2; ISSN: 1005-1511
PUBLISHER: Hecheng Huaxue Bianjibu
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
OTHER SOURCE(S): CASREACT 134:131271
AB A convenient route for the synthesis of liq. crystal compd. 4-(trans-4-pentylcyclohexyl)-4'-(trans-4-propylcyclohexyl)-1,1'-biphenyl by reaction of 4-(trans-4-propylcyclohexyl)phenylboronic acid with 1-bromo-4-(trans-4-pentylcyclohexyl)benzene is described. The reaction is catalyzed by PdCl2 in the presence of cetrimonium bromide as a PTC under ultrasound irradn. for 20 min at room temp. The conversion of the reaction is 97% with selectivity 62% at the product purity 95%. The structure of the product is confirmed by IR, 1H NMR and MS spectra. The DSC measurement of the title compd. showed that its phase transition temp. is 57.degree.C .apprx. 312.degree.C from m.p. to isotropy.

L49 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1995:538440 HCAPLUS
DOCUMENT NUMBER: 122:285665
TITLE: Boronic acid adducts of rhenium dioxime and technetium-99m dioxime complexes containing a biochemically active group useful as diagnostic and therapeutic agents
INVENTOR(S): Nunn, Adrian D.; Linder, Karen E.; Jurisson, Silvia; Eckelman, William C.
PATENT ASSIGNEE(S): Bracco International B.V., Neth.
SOURCE: U.S., 20 pp. Cont.-in-part of U.S. Ser. No.468, 884, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5387409	A	19950207	US 1992-818705	19920107
CA 2034042	AA	19910719	CA 1991-2034042	19910111
ZA 9100300	A	19911127	ZA 1991-300	19910115
IL 96946	A1	19951208	IL 1991-96946	19910115
IL 114175	A1	19961031	IL 1991-114175	19910115
AU 9169385	A1	19910725	AU 1991-69385	19910116
AU 651076	B2	19940714		
IN 176431	A	19960525	IN 1991-DE32	19910116
NO 9100201	A	19910719	NO 1991-201	19910117
FI 9100274	A	19910719	FI 1991-274	19910118
CN 1054070	A	19910828	CN 1991-101146	19910118
CN 1034078	B	19970219		
JP 04212099	A2	19920803	JP 1991-19465	19910118
AU 9479147	A1	19950216	AU 1994-79147	19941201
CN 1111621	A	19951115	CN 1995-103488	19950322
CN 1120437	A	19960417	CN 1995-109333	19950801

PRIORITY APPLN. INFO.: US 1990-466884 B2 19900118
IL 1991-96946 A3 19910115
OTHER SOURCE(S): MARPAT 122:285665
AB Boronic acid adducts of technetium-99m and radioactive rhenium dioxime complexes, each of which include biochem. active groups, are useful as diagnostic and therapeutic agents, resp. The complexes of the invention have the formula MX(Y3)Z [M = Tc radionuclide or Re radionuclide; X = anion; Y = vicinal dioxime HON:C(R1)C(R2):NOH (R1, R2 = H, halo, alkyl, aryl, etc.); Z = boron deriv. B(A1)pR3 (R3 is or contains a biochem. active group; (A1)p is absent when p = 0 or spacer when p .gtoreq. 1 (A1 = CH2, CH:CH:, cycloalkyl, aryl, heterocyclo, etc.))]. The biochem. active

group may be mols. with an affinity for a steroid receptor, sugars, barbiturates, antihypertensives, substrates for dopamine receptors, etc. Prepn. of the compds. of the invention is included. Also reported are lung uptake data for 99mTc complexes contg. e.g. dimethylglyoxime and 4-[2-((1-methylethyl)amino)**propyl**]**phenyl** **boronic** acid.

L49 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1994:695736 HCAPLUS
DOCUMENT NUMBER: 121:295736
TITLE: Probing the specificity of the S1 binding site of subtilisin Carlsberg with boronic acids
AUTHOR(S): Seufer-Wasserthal, Peter; Martichonok, Valeri; Keller, Thomas H.; Chin, Bain; Martin, Richard; Jones, J. - Bryan
CORPORATE SOURCE: Dep. Chem., Univ. Toronto, Toronto, M5S 1A1, Can.
SOURCE: Bioorganic & Medicinal Chemistry (1994), 2(1), 35-48
CODEN: BMECEP; ISSN: 0968-0896
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A range of aryl and arylalkyl boronic acids has been prepd. and evaluated as inhibitors of the serine protease subtilisin Carlsberg, with the goal of exploring the factors controlling binding to the S1 site.

L49 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1991:509152 HCAPLUS
DOCUMENT NUMBER: 115:109152
TITLE: Probing the specificity of the S1 binding site of subtilisin Carlsberg with boronic acids
AUTHOR(S): Keller, Thomas H.; Seufer-Wasserthal, Peter; Jones, J. Bryan
CORPORATE SOURCE: Dep. Chem., Univ. Toronto, Toronto, ON, M5S 1A1, Can.
SOURCE: Biochemical and Biophysical Research Communications (1991), 176(1), 401-5
CODEN: BBRCA9; ISSN: 0006-291X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The binding properties and limitations of the key S1 site of subtilisin Carlsberg were probed with boronic acid inhibitors bearing structurally varied substituents ranging from small alkyl to large arom. groups. The data permitted structural features favoring, and disfavoring, good S1 binding to be clarified. In addn., applications of electrostatic energy calcns. identified a hitherto unsuspected region of pos. potential in the fundamentally hydrophobic S1 pocket, whose interactions with electroneg. substituents of inhibitors can make significant binding contributions.

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ACCESSION NUMBER: 1961:53956 HCAPLUS
DOCUMENT NUMBER: 55:53956
ORIGINAL REFERENCE NO.: 55:10320d-f
TITLE: Aliphatic borohydrocarbons
INVENTOR(S): Koster, Roland
PATENT ASSIGNEE(S): Studiengesellschaft Kohle m. b. H.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1056126		19590430	DE	
GB 852488			GB	
GB 852488			GB	

US 3287415 1966 US

AB The title compds. were prepd. by reaction of tri-N-alkylborazines with olefins in the absence of O and H2O at 130-60.degree. in the presence of a solvent, e.g. satd. aliphatic or aromatic hydrocarbons, ethers, or tertiary amines, if necessary under raised pressure. 1-Decene (426 g.) was heated under N with stirring to 120-30.degree. and within 30 min. 115 g. tri-N-ethylborazine added; Et3N (I) was split off and distd. during the reaction. After heating 1 hr. to 130-40.degree., the residual I was distd. in vacuo and 440 g. tridecylboron remained, a viscous oil, in quant. yield. Analogously were prepd.: Et3B, b. 94-5.degree.; tricyclohexylboron, m. 114-15.degree.; tricycloheptylboron, m. 100-1.degree.; tris(2-**phenyl-propyl**)**boron**; tributenyl **boron**, b0.2-0.3 70-80.degree., flammable in the presence of air; and C12H21B, b10 130-1.degree., in 95% yield from trans,trans,trans-1,5,9-cyclododecatriene.